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SOME MATHEMATICAL MODELS ARISING IN NANO- AND BIO-TECHNOLOGY

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In this thesis, three mechanical models arising from nanoscale and biological systems are investigated, namely the dynamics of various nanostructures, the axial buckling of carbon nanotubes and nanopeapods, and the worm-like chain model for stretched semi-flexible molecules and the utilization of such a model for investigating molecular stretching in the connective tissue extracellular matrix. In nanomechanics, we investigate the motion of both a carbon atom inside a carbon nanotube and a C_{60} fullerene inside a carbon nanotube [4]. We assume a continuous model for which the atoms are assumed to be smeared across the surface of the molecule, so that the pairwise molecular energy can be approximated by performing surface integrals. The spiral path of the atom is found to be stable, but the spiral path of the C_{60} fullerene is shown to only exist for a few picoseconds. Next, we investigate the motion of a nanoscale tippe top spinning on the interior of a single-walled carbon nanotube in the presence of a variable magnetic field [5]. Unlike the classical tippe top, the nanoscale tippe top does not flip over since the gravitational effect is insignificant at the nanoscale. After the precession, if we apply an opposite retarding magnetic force at the contact point, then the molecule will return to its original standing position. We next investigate some nanoscale orbiting systems; in particular, we study an atom and a C_{60} fullerene orbiting around a single infinitely long carbon nanotube and a C_{60} fullerene orbiting around a C_{1500} fullerene [3]. We find that the circular orbiting frequencies of the proposed nanosystems are in the gigahertz range and the classification of their orbiting paths is determined numerically.

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For the axial buckling of carbon nanotubes and nanopeapods, we investigate the buckling behavior of doubly clamped multi-walled carbon nanotubes and nanopeapods as nanoelectromechanical systems. We incorporate the bending curvature of the tube into the elastic energy and determine the nanotubes' maximum displacement for all bending regimes. We find that while the approximate solution (without curvature) underestimates the maximum displacement of the buckled carbon nanotube in the weak bending regime, our numerical solution provides an entirely different prediction in comparison to the approximate solution in the strong bending regime. Furthermore, we derive an instability condition for multi-walled carbon nanotubes and nanopeapods under an axial load by taking into account the van der Waals forces between molecules. We observe that the critical force derived from the axial buckling stability criterion decreases as a result of the molecular interactions between adjacent layers of the nanotubes and the molecular interactions between the embedded fullerenes and the inner carbon nanotube.

The worm-like chain model arises as a model for stretched semi-flexible molecules and for its applications to molecular stretching in the extracellular matrix; we adopt a variational principle to examine the model [2] and then utilize the model to describe anionic glycosaminoglycan between collagens. The worm-like chain model has been proposed assuming that each monomer resists the bending force. We determine a force-extension formula for the worm-like chain model analytically, and find that our formula suggests new terms such as the free energy and the cut-off force for a molecule. In addition, we predict two possible phase changes for a stretched molecule, and show theoretically that a molecule must undergo two phase changes when they are stretched beyond their total contour lengths. Furthermore, we adopt the worm-like chain model to describe the mechanical properties of a collagen pair in the connective tissue extracellular matrix [1]. We find that the growth of fibrils is intimately related to the maximum length of the anionic glycosaminoglycan and the relative displacement of two adjacent fibrils.

References

[1] Y. Chan, G. M. Cox, R. G. Haverkamp and J. M. Hill, 'Mechanical model for a collagen fibril pair in extracellular matrix', *Eur. Biophys. J.* **38** (2009), 487–493.

[2] Y. Chan, R. G. Haverkamp and J. M. Hill, 'Force-extension formula for the worm-like chain model from a variational principle', *J. Theoret. Biol.* **262** (2010), 498–504.

[3] Y. Chan, N. Thamwattana, G. M. Cox and J. M. Hill, 'Mechanics of nanoscale orbiting systems', *J. Math. Chem.* **46** (2009), 1271–1291.

[4] Y. Chan, N. Thamwattana and J. M. Hill, 'Spiral motion of carbon atoms and C_{60} fullerenes inside single-walled carbon nanotubes', *Int. J. Theor. Appl. Multiscale Mechanics* **1** (2009), 176–192.

[5] Y. Chan, N. Thamwattana and J. M. Hill, 'Magnetic field driven nano tippe top', *J. Comput. Theor. Nanosci.* **6** (2009), 1013–1020.

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