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PREDICTING PIEZOELECTRIC EFFECTS IN ATOMISTIC FINITE ELEMENT SIMULATIONS

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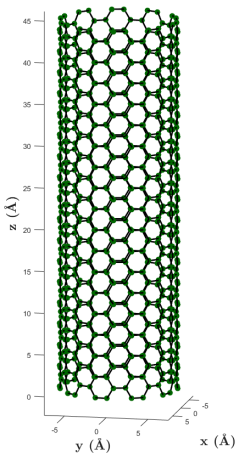
Summary As our ability to build ever smaller machines develops so does the need for simulation techniques that can accurately capture the behaviour of these nanocomponents. To empower designers, new simulation methods must be developed to allow for easy and fast iterations of designs. To this end we have sought to incorporate piezoelectric modelling within an atomistic finite element model of boron nitride nanotubes. The ability to capture these effects allows for the design of nano scale electromechanical devices. We built and tested the model by using it to calculate the piezoelectric tensor coefficients for armchair boron nitride nanotubes, subjected to an axial torsional loading and compared our values to those generated using density functional theory that are available in the literature.

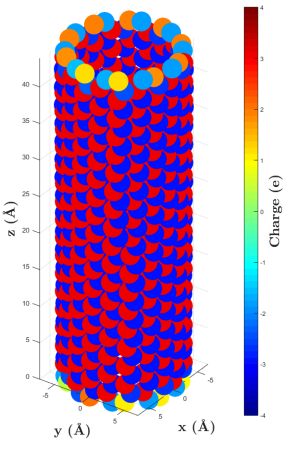
INTRODUCTION

Interest in nanotubes and their potential applications has been growing ever since their initial prediction over two decades ago. Different materials have been investigated as potential candidates for nanotube formation starting with the most well known, carbon, but other materials such as carbon nitrides, boron nitrides, sulphides, selenides, halides and transition metal oxides have been investigated [1]. Concurrently, there has been development of micro, meso and nano scale machines looking to provide new technological capabilities in many different research fields. Components of these miniature machines are an obvious application for nanotubes, however new methods for accurately modelling these structures are required. The standard methods for macro scale modelling rely on the assumptions of continuum mechanics, where as at smaller scales the molecular structure of the materials becomes apparent leading to unacceptable inaccuracies. Although computational chemistry has produced tools for modelling molecular structures they normally require significant computational resources when attempting to model large systems of atoms. One method that attempts to provide molecular modelling capabilities while allowing for rapid computation is to model the molecular structure as a space frame structure (as can be seen in figure 1a) by using force constants developed for molecular mechanics software to provide the effective beam (Euler-Bernoulli or Timoshenko) properties [2]. These "atomistic" finite element models have been investigated for over a decade by multiple authors, examining different nano materials and using different finite element beam formulations [3, 4, 5].

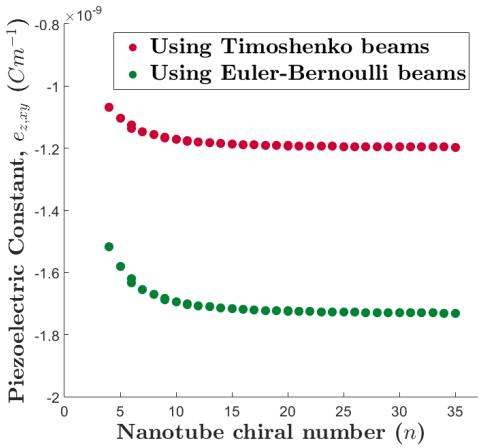
We want to expand this technique by providing a method for calculating properties other than the mechanical ones that have been investigated previously. The focus of this work was on developing a novel method for calculating the piezoelectric response of nanotubes. Boron nitride nanotubes have been shown to have piezoelectric properties which have been investigated, mostly computationally, providing us with a means for testing the validity of our method.



(a) The finite element model of a nanotube showing beam elements as black lines and the nodes as green circles.



(b) The charges of the atoms of the boron nitride nanotube as calculated using QEq.



(c) The results of our simulations showing a similar trend in the piezoelectric coefficient as the nanotube chiral number (an analogue for the tube radius) is increased.

Figure 1

THE METHOD

Piezoelectric phenomena are generated by the creation of atomic dipoles in a material which are at least somewhat aligned. In the case of boron nitride nanotubes the atomic dipoles are caused by distortions of the nanotube lattice that result in breaking of the threefold symmetry of the lattice. This symmetry breaking leads to dipole creation whereby the electron distribution of the atoms loses symmetry resulting in a dipole moment of the atom.

A simple method for understanding this behaviour is to consider a polarisability of the atom, a constant which describes the ratio of the dipole moment of the atom generated by an external applied field and the strength of the applied field. Using atomic polarisability we can calculate the dipole moment of an atom due to an applied field, for our purposes it was thus necessary to find a suitable method for calculating the electric field at the atom sites of our deformed nanotube lattice.

The method we used was one developed for use with molecular mechanics simulations called charge equilibration (QEq). This method uses physical properties of the atoms, the ionisation energies and electron affinities, and the atom positions as the initial inputs for a method to approximate the charge distribution within a molecule (an example of which can be seen in figure 1b). Using this method we were able to generate charges for the atoms in the deformed nanotube and then use these charges and the position data for the atoms to calculate the electric field at the atom sites. With the field calculated we could then apply the polarisability to find the dipole moments of the atoms.

TESTING THE METHOD

To determine the accuracy of the method we chose to generate the piezoelectric coupling tensor coefficients of a variety of different sized armchair boron nitride nanotubes under an axial shear load (for results see figure 1c). By varying the degree of the shear stress in the tube due we could calculate the dipole moment per unit area (dipole density) of the tube for each applied shear stress. We were then able to find the gradient of the dipole density as a function of shear stress using finite differences. This gradient is the tensor coefficient for the piezoelectric coupling tensor.

Table 1: Results from our model and other authors work.

Authors	Method	$e_{z,xy}$ (Cm^{-1})
Current work	Atomistic FE with QEq	-1.46×10^{-9}
Sai & Mele [6]	DFT/Berry's phase	-3.63×10^{-10}
	DFT/Ab initio	-2.60×10^{-10}
Naumov et al [7]	DFT	-3.57×10^{-10}

Our results show reasonable agreement with calculations for the tensor values based on DFT calculations (see table 1) but further refinement of the method is required. Future work will seek to address this by examining other piezoelectric nanotubes, such as zinc oxide, so that suitable corrections can be introduced to the relevant physical constants.

CONCLUSIONS

We developed and tested a method for the simulating piezoelectric response of boron nitride nanotubes. The method provides us with an approximation of the piezoelectric properties of the nanotubes but will be refined through future work. We have shown the method has potential to be used for simulating nanostructures and therefore has the potential to be used as a tool for designing nano scale machines that utilise piezoelectric effects that are present in certain materials.

References

[1] V V Pokropivnyi. Non-carbon nanotubes (review). II. types and structure. *Powder metallurgy and metal ceramics*, 40(422):582–594, 2001.

[2] Chunyu Li and Tsu-Wei Chou. A structural mechanics approach for the analysis of carbon nanotubes. *International Journal of Solids and Structures*, 40(10):2487–2499, may 2003.

[3] K. I. Tserpes and P. Papanikos. Finite element modeling of single-walled carbon nanotubes. *Composites Part B: Engineering*, 36(5):468–477, 2005.

[4] F Scarpa, S Adhikari, and A Srikantha Phani. Effective elastic mechanical properties of single layer graphene sheets. *Nanotechnology*, 20(6):065709, 2009.

[5] M Meo and M Rossi. Prediction of Youngs modulus of single wall carbon nanotubes by molecular-mechanics based finite element modelling. *Composites Science and Technology*, 66(11-12):1597–1605, 2006.

[6] Na Sai and E. J. Mele. Microscopic theory for nanotube piezoelectricity. *Physical Review B*, 68(24):241405, dec 2003.

[7] Ivan Naumov, Alexander M. Bratkovsky, and V. Ranjan. Unusual Flexoelectric Effect in Two-Dimensional Noncentrosymmetric sp^{2}-Bonded Crystals. *Physical Review Letters*, 102(21):217601, 2009.