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QUALITATIVE INTERPRETATION OF CARBON NANOTUBE BY USING THE MODELLING OF ATOMIC CHAIN AS A COSSERAT CURVE

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ABSTRACT

This paper studies the mechanical properties of carbon nanotubes by an atom chain modelling through a Corresat curve theory. The Cauchy-Born rule is applied for spanning multi-scales from atomistic field to macroscopic space. A one-dimensional Cosserat theory is adopted where a displacement field-independent rotation tensor is introduced, which describes the rotation of the inner structure. Empirical interatomic potentials are employed for the calculations of the displacement and modulus fields. Simulations are achieved by a finite element approach. The results have shown that the atom chain model is capable to interpret the behaviours of carbon nanotubes qualitatively.

Keywords: carbon nanotube, atomic chain, Cauchy-Born rule, Cosserat curve, empirical interatomic potential.

INTRODUCTION

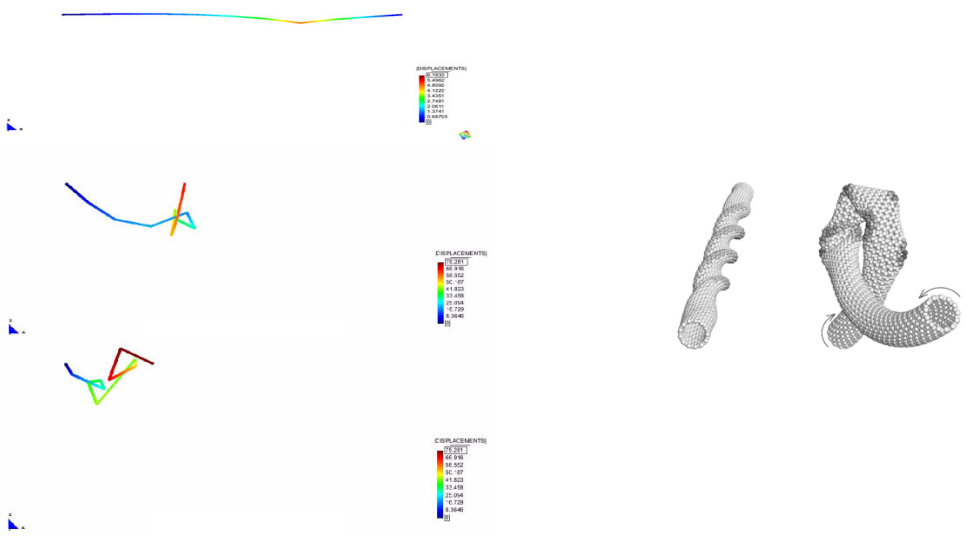
It was a revolution in nano-science when carbon nanotubes (CNTs) were discovered with their outstanding properties (Iijima, 1991). Because of their unique electrical properties and extremely high thermal conductivity, CNTs have been used for electronics, field-emission displays, energy storage, functional fillers in composites, and some biomedical devices.

The mechanical properties of CNTs have been studied worldwide by scientists and engineers since. However, a robust, theoretically precise and computationally efficient prediction method of the mechanical properties of CNTs has not yet been found. Continuum shell theory has been applied extensively to model CNTs (Arroyo, 2004). Only in recent years, continuum rod theory has been developed for the study of CNTs. For instance, Chandraseker (2009) modelled a single-walled CNT as a Cosserat rod with finite thickness bounded by the lateral surface. As an extension, Kumar (2011) studied three-dimensional deformations of single-walled CNTs via a Cosserat rod theory.

This paper develops a new atomistic and continuum mixing modelling technique, where the Cauchy-Born rule is applied to link the micro-space to the macro-space, the constitutive laws are derived from empirical atomistic potentials which deal with individual interactions between single atoms at the micro-level, and a Cosserat curve theory is adopted to describe the averaged behaviour of a CNT at the macro-level. The mixing method is more computationally practical than atomistic simulations and can provide more accurate physical results than classical continuum methods.

RESULTS AND CONCLUSIONS

The Cosserat curve simulation result shows, after the instant disturbance, that the thread tends to vibrate about a random weak spot with small amplitude. Fig. 1(a) demonstrates the simulation of thread coiling after the disturbance, with the pushing load applied, with both rotating and twisting deformations. It matches the simulation results of the torsion of CNTs by Yakobson (1996) using atomistic methods, where the deformation pattern changed from a straight spiral to sideways buckling and then coils into a loop, as shown in Fig. 1(b).



(a) (b)

Fig. 1 - Simulation of torsion of CNT by: (a) Cosserat curve theory; (b) atomistic simulation (Yakobson, 1996)

From the results, it is shown that, since it brings a great advantage over atomistic methods with much less computational efforts on a large scale of CNTs, an atomic chain model can be a qualitative model of CNT when it is considered as a Cosserat curve.

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