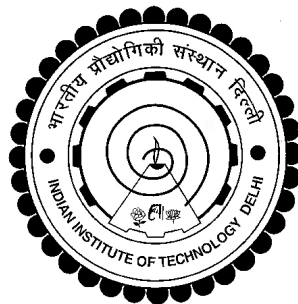


ELASTICITY OF ONE-DIMENSIONAL NANOSTRUCTURES - A MULTISCALE APPROACH

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INDIAN INSTITUTE OF TECHNOLOGY DELHI
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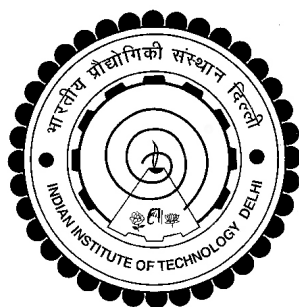
by

PRAKHAR GUPTA

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Submitted

in fulfillment of the requirements of the degree of Doctor of Philosophy
to the



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MAY 2018

Certificate

This is to certify that the thesis entitled “**Elasticity of one-dimensional nanostructures - a multiscale approach**”, being submitted by **Prakhar Gupta** to the Indian Institute of Technology Delhi for the award of the degree of **Doctor of Philosophy**, is a record of the bonafide research carried out by him which has been prepared under my supervision in conformity with the rules and regulations of the Indian Institute of Technology Delhi. The research reports and results presented in the thesis has not been submitted for any degree or diploma in any other university or institute.

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Abstract

Interest in one-dimensional nanostructures (e.g., carbon nanotubes, DNA, nanorods etc.) has surged dramatically due to their exceptional optical, thermal, electrical, magnetic and mechanical properties. The deformations of these nanostructures have been studied using both fully molecular approach as well as continuum formulations. These nanostructures have been modeled using two-dimensional shell theory as well as several one-dimensional theories such as Euler-Bernoulli and Timoshenko beam theories. However, the one-dimensional theories fail to model large cross-sectional rotation in these nanostructures. To overcome this limitation, this thesis focusses on modeling of elasticity of such nanostructures using the one-dimensional continuum theory of Cosserat rods.

Broadly speaking, the present work proposes three different techniques to obtain nonlinear elastic constitutive relations of these nanostructures: (1) a multiscale technique (*Helical cauchy-Born* rule) to obtain nonlinear elastic constitutive relations through molecular statics of the smallest repeating cell of nanostructures (2) a fully continuum approach to obtain extensional and twisting stiffnesses of circular nanorods incorporating also the surface effects (3) use of phonon dispersion curves to obtain stiffnesses.

Using the *Helical Cauchy-Born (HCB)* rule, shearing stiffness and several other coupling stiffnesses of nanorods (e.g., coupling between bending-shear, bending-stretching, bending-twisting etc.) can now be obtained accurately when compared to existing techniques. The stiffnesses so obtained do not obey the usual formulae for continuum beams primarily due to surface stress effects inherent in nanobeams. To capture this effect in a fully continuum-setting, explicit analytical formulae for extensional and twisting stiff-

nesses of isotropic circular nanorods are also obtain in terms of their bulk and surface material constants. The continuum formulae for stiffnesses of rectangular nanorods already exist in the literature. These formulae have however been incorrectly extended by various researchers to circular nanorods. Our formulae suggest that these stiffnesses not only depend upon surface and bulk elastic constants but also on surface residual stress. Finally, we discuss about phonons in the context of chiral nanotubes and show how phonon dispersion data can be used to obtain various stiffnesses of chiral nanotubes. We also obtain analytical formulae to show the effect of coupling stiffnesses as well as stretching and twisting of the nanotube on frequencies as well as mode shapes of longitudinal, torsional, bending, shearing and radial breathing phonon modes. Existing works in this regard are very limited.

These methods are used to obtain various stiffnesses of diamond nanorods, tungsten nanorods and single walled carbon nanotubes (SWCNTs) when modeled as a special Cosserat rod. It is shown that the extensional and twisting stiffnesses of circular tungsten nanorods obtained using the HCB rule follow our analytical formulae for stiffnesses accurately. We also obtain interesting buckling results for diamond nanorods and SWCNTs using fully atomistic simulations. These observations from fully atomistic simulations are accurately replicated in the finite element special Cosserat rod simulation when the material nonlinearity is also incorporated. However, the FEM results exhibit completely different trend when only linear material laws are incorporated.

सार

एकविमीय अतिसूक्ष्म संरचनाओं (जैसे, कार्बन की अतिसूक्ष्म नलिकाएं, डीएनए, अतिसूक्ष्म छड़ इत्यादि) में रुचि उनके असाधारण, प्रकाशीय, उष्ण, विद्युत, चुंबकीय और यांत्रिक गुणों के कारण बढ़ी है। इन अतिसूक्ष्म संरचनाओं के विकृतियों का अध्ययन करने के लिए आणविक दृष्टिकोण के साथ-साथ संतात्यक सूत्रीकरण का उपयोग किया गया है। इन अतिसूक्ष्म संरचनाओं को द्विविमीय खोल सिद्धांत के साथ-साथ कई एकविमीय जैसे यूलर-बर्नौली और तिमोशेन्को बीम सिद्धांतों का उपयोग करके प्रतिरूपण किया है। हालांकि, एकविमीय सिद्धांत इन अतिसूक्ष्म संरचनाओं में बड़े पार अनुभागीय नियमित आवर्तन का प्रतिरूप करने में असफल हो जाते हैं। इस कमी को दूर करने के लिए, यह शोध-प्रबन्ध एकविमीय कोसराट छड़ सिद्धांत के माध्यम से अतिसूक्ष्म संरचनाओं की प्रत्यास्थता के प्रतिरूपण पर केंद्रित है।

वर्तमान लेखन इन अतिसूक्ष्म संरचनाओं के अरेखीय प्रतिबल - विकृति सम्बन्ध में तीन तकनीकें प्रस्तुत करता है: (१) एक बहुपैमानिय तकनीक (हेलिकल कौची-बोर्न नियम) के माध्यम से अतिसूक्ष्म संरचना के सबसे छोटे दोहराने वाले कक्ष की आणविक स्थैतिक के द्वारा अरेखीय प्रतिबल - विकृति सम्बन्ध प्राप्त करना (२) संतात्यक दृष्टिकोण के माध्यम से खिंचाव और मरोड़ दुर्नम्यता प्राप्त करना जिसमें सतह प्रभाव भी शामिल हैं (३) फोनन फैलाव वक्र के माध्यम से दुर्नम्यता प्राप्त करना।

मौजूदा तकनीकों की तुलना में हेलिकल कौची-बोर्न (एच.सी.बी.) नियम का उपयोग करते हुए, अब अपरूपण दुर्नम्यता एवं अन्य युग्मन दुर्नम्यता (उदाहरण के लिए, बंकन - अपरूपण, बंकन -खिंचाव, बंकन -मरोड़ आदि के बीच युग्मन) सटीक रूप से प्राप्त किये जा सकते हैं। प्राप्त की गई दुर्नम्यता अतिसूक्ष्म छड़ में अंतर्निहित पृष्ठ प्रतिबल के कारण संतात्यक छड़ के सामान्य सूत्रों का पालन नहीं करती है। इस प्रभाव को संतात्यक स्थापना में शामिल करने के लिए, समदैशिक वृत्तीय अतिसूक्ष्म छड़ के खिंचाव और मरोड़ स्टिफनेस के लिए विश्लेषणात्मक सूत्र भी प्राप्त किये गए हैं। आयताकार अतिसूक्ष्म छड़ की दुर्नम्यता के सांतत्यक सूत्र पहले से ही साहित्य में मौजूद हैं। परन्तु यह सांतत्यक सूत्र शोधकर्ताओं ने गलत रूप से वृत्तीय अतिसूक्ष्म छड़ के लिए भी विस्तृत किया है। हमारे द्वारा प्राप्त किये गए सूत्र न केवल बल्क और पृष्ठ प्रत्यास्थता पर निर्भर करते हैं बल्कि पृष्ठ अवशिष्ट प्रतिबल पर भी निर्भर करते हैं। अंत में, हम काइरल अतिसूक्ष्म नलिकाओं के संदर्भ में फोनन के बारे में चर्चा करते हैं जिसमें काइरल अतिसूक्ष्म नलिकाओं की विभिन्न दुर्नम्यता प्राप्त करने के लिए फोनन फैलाव वक्र का उपयोग किया जा सकता है। युग्मन दुर्नम्यता के साथ-साथ अतिसूक्ष्म नलिका के खिंचाव और मरोड़ का प्रभाव आवृत्ति पर एवं अनुदैर्घ्य, मरोड़, बंकन, कर्तन और अरीय श्वास फोनोन मोड पर विश्लेषणात्मक सूत्र के माध्यम से प्रदर्शित किया है। इस संबंध में मौजूदा काम बहुत सीमित हैं।

जब विशेष कोसराट छड़ के रूप में हीरा, टंगस्टन के अतिसूक्ष्म छड़ और कार्बन की अतिसूक्ष्म नलिका (एसडब्ल्यूसीएनटी) का प्रतिरूपण किया तब इन तरीकों से इनकी विभिन्न दुर्नम्यता प्राप्त की गई हैं। हमारे द्वारा प्राप्त खिंचाव और मरोड़ दुर्नम्यता के विश्लेषणात्मक सूत्र वृत्तीय टंगस्टन अतिसूक्ष्म छड़ के लिए एच.सी.बी. नियम से मेल खाते हैं। परमाणवीय सिमुलेशन का उपयोग करते हुए हीरा अतिसूक्ष्म छड़ और एसडब्ल्यूसीएनटी के लिए दिलचस्प व्याकुंचन परिणाम भी प्राप्त किये गए हैं। जब असमानुपातिक प्रतिबल – विकृति सम्बन्ध परिमित अवयव स्पेशल कोसराट छड़ सिमुलेशन में सम्मिलित किये जाते हैं तब वह परमाणवीय सिमुलेशन के द्वारा प्राप्त किये गए परिणाम से मेल खाते हैं। हालांकि, परिमित अवयव परिणाम पूरी तरह अलग प्रदर्शित होते हैं जब सामान्य प्रतिबल – विकृति सम्बन्ध शामिल किया जाता है।

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