

THERMOELASTOPLASTIC MODELING OF ONE DIMENSIONAL STRUCTURES

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**DEPARTMENT OF APPLIED MECHANICS
INDIAN INSTITUTE OF TECHNOLOGY DELHI
OCTOBER 2020**

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**THERMOELASTOPLASTIC MODELING OF ONE
DIMENSIONAL STRUCTURES**

by

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Department of Applied Mechanics

Submitted

in fulfilment of the requirements of the degree of Doctor of Philosophy

to the



INDIAN INSTITUTE OF TECHNOLOGY DELHI

OCTOBER 2020

*Dedicated To
My Brother and My Parents*

Certificate

This is to certify that the thesis entitled “**Thermoelastoplastic modeling of one dimensional structures**”, being submitted by Ms. **Smriti** to the Indian Institute of Technology Delhi for the award of the degree of **Doctor of Philosophy**, is a record of bonafide research carried out by her under my supervision. The thesis in my opinion, is worthy of consideration in accordance with the rules and regulations of the Institute. To the best of my knowledge, the results embodied in this thesis have not been submitted to any other University or Institute for the award of any other degree or diploma.

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Acknowledgements

I wish to express my heartiest gratitude to my supervisor Professor Ajeet Kumar, Department of Applied Mechanics, IIT Delhi, for his precious suggestion, encouragement and inspiring enthusiasm throughout my PhD. I am grateful to him for sharing his immense knowledge through the fruitful discussions which helped me understand this work better. I also learnt heavily from the courses that he taught us, i.e., Applied Elasticity, Advanced Solid mechanics and Multiscale Modeling. I consider myself lucky that I got this opportunity to work with him. His passion and dedication towards research is simply unmatched and this has always been a source of motivation for me. I am wholeheartedly thankful to him for giving me all the experiences to learn and grow. I would also like to express my sincere thanks to Prof. Paul Steinmann who has guided me on plasticity and encouraged me throughout my PhD Journey.

I would also like to express my gratitude to my student research committee members: Professor Rajesh Prasad, Professor Jayant Jain and Professor Devendra Dubey for their guidance and advice throughout the course of my PhD. I also express my sincere thanks to other faculty members of IIT Delhi for their constant support. My sincere thanks to all the teachers who supported me and encouraged me to pursue my dream.

I am extremely grateful to all my labmates: Darius Diogo Barreto, Dr. Prakhar Gupta, Dr. Raushan Singh, Mohit Garg, Intaf Alam, Amit Sharma, Adil Iqbal, Shashank Saxena, Jaya Tiwari, for providing a healthy environment for technical as well as non-technical discussions. I am also thankful to my other departmental colleagues: Rishi Mishra, Sagar Saroha, Nishant Parashar, Vikas Dwivedi, with whom I shared this wonderful experience. As a whole, my stay at IIT Delhi was wonderful and I would like to thank IIT Delhi for giving me this beautiful experience.

I am incredibly thankful to my parents, Mrs. Manorama Devi and Mr. Keshav Prasad for believing in me and allowing me to pursue my passion. I am extremely grateful to my brother Rahul Rajan and my sister in law Swati Rajan, who supported me unconditionally and took a very good care of the family while I was away. I am grateful to my grandfather and late grandmother for their never-ending love and blessings. It is my family who taught me the lessons on moral and spiritual values and kept inspiring me in all times. Finally, Lord, thank you for all the love and blessings.

Smriti

Abstract

Interest in the theory of rods has been the subject of intense research due to its applicability in several areas of scientific and applied research such as its applicability in biophysics, modeling chiral nanotubes, biomolecules, arteries, cables, ropes, strings etc. It is used in modeling deformation in slender bodies whose dimension in one direction is much longer compared to the other two. The theory differs from the classical beam theories such as the Euler-Bernouli and Timoshenko beam theories primarily because the latter theories are geometrically linear which can model only small rotation of the beam's cross-section. The theory of rods, on the other hand, is nonlinear and geometrically exact allowing large rotation of the cross-section which, in turn, also needs nonlinear constitutive relations when the induced curvature and twist are large enough. In the context of modeling of nanorods and notubes, if we use nanoscale experiments, we might obtain the linear moduli but not the nonlinear moduli. Alternately, one can use molecular simulation to obtain nonlinear constitutive laws. In an attempt to extract the constitutive relations for nanorods, the first part of the thesis is dedicated towards establishing a microscopic framework for one-dimensional nanostructures and thereby, deducing the expressions of their thermoelastic constants. In the second part of the thesis, we again talk about the theory of rods, but at the continuum scale. The theory of rods has been primarily used to model elastic deformations. However, we present a general framework to model their elastoplastic deformation and also present a finite element based numerical scheme.

We have presented a one-dimensional variant of the Irving-Kirkwood-Noll procedure to obtain microscopic expressions of internal contact force and moment. The derived expressions give both kinetic and potential parts of force and moment which hold also in thermodynamic nonequilibrium. We showed analytically as well as numerically that the total force must contain both potential and kinetic parts, only then it becomes analogous to the internal contact force at continuum level. We also derived expressions of extensional, torsional and bending stiffnesses but from the second derivative of Helmholtz free energy per unit length with respect to strain parameters. The expressions of stiffnesses hold only in thermodynamic equilibrium. The derived expressions were used to investigate extension, compression, torsion and bending of SWCNTs. These expressions provide us with a way to obtain internal force, moment and stiffnesses more accurately during molecular simulation - the existing approach of obtaining them by numerical differentiation of energy with respect to strain parameters is prone to numerical error. We then obtain expressions for heat capacity and thermal stress coefficients for a helically repeating nanostructure in thermodynamic equilibrium from the second derivative of Helmholtz free energy with respect to temperature and strain measures. The derived expressions are

used in molecular dynamics simulation to study the variation of thermoelastic constants with temperature in single-walled carbonnanotubes.

We then turn towards the continuum elastoplastic deformation in the context of special Cosserat rods. In this thesis, a general framework is presented to model coupled elastoplastic deformation in the theory of special Cosserat rods. The use of the one-dimensional form of the energy balance in conjunction with the one-dimensional entropy balance allows us to obtain the constitutive relations for this theory. Later on, additive decomposition is used to separate the elastic part of the strain measures of the rod from their plastic counterparts. We then present the most general quadratic form of the Helmholtz energy per unit rod's undeformed length for both hemitropic and transversely isotropic rods. We also propose a prototype yield criterion in terms of forces, moments and hardening stress resultants as well as the associative flow rules for the evolution of plastic strain measures and hardening variables. We then present a finite element formulation for the elastoplastic deformation in the special Cosserat rod theory and obtain a general elastoplastic tangent stiffness matrix. The formulation assumes the existence of a yield function in terms of stress resultants over the rod's cross-section, i.e., force, moment and hardening stress resultants. The associated flow rule is assumed for the evolution of the rod's plastic strain measures and hardening variables. A return map algorithm is developed in order to obtain consistent algorithmic elastoplastic tangent moduli of the rod. The formulation presented is used to study the combined extension-torsion loading of a straight rod with different cases of hardening. Another problem of snap-through buckling of a semi-circular arch subjected to a vertically downward load at its mid-section is also investigated. The effect of various elastoplastic parameters of the arch on its load-displacement curve are presented.

सार

वैज्ञानिक और व्यावहारिक अनुसंधान के कई क्षेत्रों में इसकी प्रयोज्यता के कारण छड़ के सिद्धांत में रुचि गहन शोध का विषय रहा है, जैसे कि जैव-भौतिकी में इसकी प्रयोज्यता, चिरल नैनोट्यूब, बायोमोलेक्यूलस, धमनियों, केबल, रस्सियों, तार आदि का मॉडलिंग। यह सिद्धांत शास्त्रीय बीम सिद्धांतों से अलग है जैसे यूलर-बर्नौली और टिमकाँइन बीम सिद्धांत, मुख्य रूप से क्योंकि बाद के सिद्धांत ज्यामितीय रूप से रैखिक हैं जो बीम के क्रॉस-सेक्शन के केवल छोटे रोटेशन को मॉडल कर सकते हैं। दूसरी ओर, छड़ का सिद्धांत, गैर-रेखीय और ज्यामितीय रूप से सटीक है जो क्रॉस-सेक्शन के बड़े रोटेशन की अनुमति देता है, जिससे जब प्रेरित वक्रता और मोड़ काफी बड़े होते हैं, तो गैर-संवैधानिक संबंधों की भी आवश्यकता होती है। नैनोरोड्स और नैनोट्यूब की मॉडलिंग के संदर्भ में अगर हम नैनोस्केल प्रयोग करते हैं, तो हम रैखिक मोडुली प्राप्त कर सकते हैं लेकिन अरेखीय मोडुली नहीं। गैर-संवैधानिक कानूनों को प्राप्त करने के लिए, वैकल्पिक रूप से, कोई आणविक सिमुलेशन का उपयोग कर सकता है। नैनोरोड्स के लिए संवैधानिक संबंधों को निकालने के प्रयास में, थीसिस का पहला भाग, उनके थर्मोइलास्टिक स्थिरांक के भावों को घटाते हुए, एक आयामी नैनोस्ट्रक्चर के लिए सूक्ष्म रूपरेखा की स्थापना के लिए समर्पित है। थीसिस के दूसरे भाग में हम फिर से बात करते हैं छड़ के सिद्धांत के बारे में, लेकिन सातत्य पैमाने पर। छड़ के सिद्धांत का मुख्य रूप से लोचदार विकृतियों को मॉडल करने के लिए उपयोग किया गया है। हालांकि, हम उनके इलास्टोप्लास्टिक विरूपण मॉडल के लिए एक सामान्य रूपरेखा प्रस्तुत करते हैं और एक परिमित तत्व आधारित संख्यात्मक योजना भी प्रस्तुत करते हैं।

हमने आंतरिक संपर्क बल और क्षण की सूक्ष्म अभिव्यक्ति प्राप्त करने के लिए इरविंग-किर्कवुड-नोल प्रक्रिया के एक आयामी संस्करण को प्रस्तुत किया है। व्युत्पन्न अभिव्यक्तियाँ बल और गति के गतिज और संभावित दोनों भागों को प्रदान करती हैं जो थर्मोडायनामिक नोक्विलीब्रियम में भी पकड़ में आती हैं। हमने विश्लेषणात्मक रूप से और साथ ही संख्यात्मक रूप से दिखाया कि कुल बल में संभावित और गतिज दोनों भाग होने चाहिए, तभी यह निरंतर संपर्क स्तर पर आंतरिक संपर्क बल के

अनुरूप हो जाता है। हमने खिचाव, टॉर्सनल और झुकने वाली कठोरता के भी भाव निकाले हैं लेकिन हेल्महोल्ट्ज़ मुक्त ऊर्जा प्रति यूनिट लंबाई के दूसरे व्युत्पन्न से। कठोरता के भाव केवल थर्मोडायनेमिक संतुलन में पकड़ रखते हैं। व्युत्पन्न अभिव्यक्तियों का उपयोग एकल दीवार वाले कार्बन नैनोट्यूब के विस्तार, संपीड़न, मरोड़ और झुकने की जांच के लिए किया गया था।

ये भाव हमें आणविक सिमुलेशन के दौरान आंतरिक बल, गति और कठोरता प्राप्त करने के तरीके अधिक सटीकता के साथ प्रदान करते हैं। तनाव मापदंडों के संबंध में ऊर्जा के संख्यात्मक विभेदन द्वारा उन्हें प्राप्त करने का मौजूदा तरीका संख्यात्मक त्रुटि के लिए प्रवण है। फिर हम हेल्महोल्ट्ज़ के दूसरे व्युत्पन्न से ऊष्मागतिकीय संतुलन में एक हेल्लो रिपीटेड नैनोसंरचना के लिए ऊष्मा क्षमता और तापीय तनाव गुणांक के लिए भाव प्राप्त करते हैं। व्युत्पन्न अभिव्यक्तियों का उपयोग एकल-दीवार वाले कार्बननोट्यूब में तापमान के साथ थर्मोइलास्टिक स्थिरांक की भिन्नता का अध्ययन करने के लिए, आणविक गतिशीलता सिमुलेशन में किया जाता है।

हम फिर विशेष कोसेराट छड़ के संदर्भ में सातत्य इलास्टोप्लास्टिक विरूपण की ओर मुड़ते हैं। इस थीसिस में, विशेष कॉज़रैट रॉड्स के सिद्धांत में इलास्टोप्लास्टिक विरूपण युग्मित मॉडल के लिए एक सामान्य रूपरेखा प्रस्तुत की जाती है। एक-आयामी एन्ट्रॉपी संतुलन के साथ संयोजन में एक-आयामी ऊर्जा संतुलन के रूप का उपयोग

हमें इस सिद्धांत के लिए संवैधानिक संबंध प्राप्त करने की अनुमति देता है। बाद में, छड़ के तनाव उपायों के लोचदार हिस्से को उनके प्लास्टिक समकक्षों से अलग करने के लिए योज्य विघटन का उपयोग किया जाता है। हम हेमट्रोपिक और ट्रांसवर्सली आइसोट्रोपिक छड़ दोनों के लिए हेल्महोल्ट्ज़ ऊर्जा प्रति यूनिट रॉड की अविकसित लंबाई के सबसे सामान्य द्विघात रूप प्रस्तुत करते हैं। हम बलों, क्षणों, और सख्त तनाव के परिणाम के संदर्भ में एक प्रोटोटाइप उपज मानदंड भी प्रस्तावित करते हैं और साथ-साथ प्लास्टिक स्ट्रेन के उपाय और सख्त चर के विकास के प्रवाह के लिए सहयोगी प्रवाह नियम प्रस्तावित करते हैं। हम तब विशेष कॉससेट रॉड सिद्धांत में इलास्टोप्लास्टिक विरूपण के लिए एक परिमित तत्व तैयार करते हैं और एक सामान्य इलास्टोप्लास्टिक स्पर्शरेखा कठोरता मैट्रिक्स प्राप्त करते हैं। यह सूत्रीकरण रॉड के क्रॉस-सेक्शन में तनाव के परिणाम यानी, बल, पल और सख्त तनाव परिणाम के संदर्भ में एक उपज समारोह के अस्तित्व को मानता है। रॉड के प्लास्टिक स्ट्रेन उपायों और सख्त चर के विकास के लिए संबंधित प्रवाह नियम मान लिया गया है। रॉड के

सुसंगत एल्गोरिथ्म इलास्टोप्लास्टिक स्पर्शरेखा प्राप्त करने के लिए, एक वापसी नक्शा एल्गोरिदम विकसित किया गया है। प्रस्तुत सूत्रीकरण का उपयोग, सख्त होने के अलग-अलग मामलों के साथ एक सीधी रॉड के संयुक्त विस्तार मरोड़ लोडिंग का अध्ययन करने के लिए किया जाता है। स्नैप-थू बकलिंग ऑफ़ सेमी-सर्कुलर आर्क की एक और समस्या, जो एक लंबवत डाउनवर्ड लोड के अधीन है, की भी जांच की जाती है। इसके लोड-विस्थापन वक्र पर विभिन्न इलास्टोप्लास्टिक मापदंडों का प्रभाव प्रस्तुत किए जाते हैं।

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