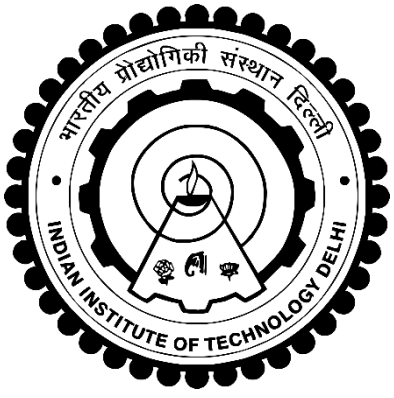
MODELLING OF NANOSTRUCTURES USING SECOND-ORDER STRAIN GRADIENT NONLOCAL THEORY

BISHWESHWAR BABU



DEPARTMENT OF APPLIED MECHANICS
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MODELLING OF NANOSTRUCTURES USING SECOND-ORDER STRAIN GRADIENT NONLOCAL THEORY

by

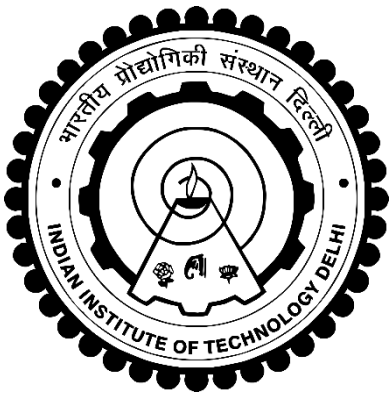
BISHWESHWAR BABU

Department of Applied Mechanics

Submitted

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

to the



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Certificate

This is to certify that the thesis entitled **"Modelling of Nanostructures Using Second-Order Strain Gradient Nonlocal Theory"** being submitted by **Mr. Bishweshwar Babu** to the Indian Institute of Technology Delhi for the award of degree of **Doctor of Philosophy** in Applied Mechanics is a record of original, bonafide record of research work carried out by him under my supervision and guidance. The thesis work, in my opinion, has reached the requisite standard fulfilling the requirements for the degree of Doctor of Philosophy.

The results contained in this thesis have not been submitted in part or in full, to any other university or institute for the award of any degree or diploma.

Date: August , 2019

Place: New Delhi

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(Bishweshwar Babu)

Abstract

Modified continuum theories are needed to capture the size effects at micro/nano scale which are not accounted for by the classical theories in the absence of any internal length scale parameter. It is concluded from the literature review that the second-order strain gradient theories include only one nonlocal parameter and are capable of representing consistent nonlocal effect for different loading/boundary conditions. Analytical solutions for nonlocal beams/plates with different boundary conditions incorporating the strain gradient effect are not available in the literature. Further, there is a need to develop computationally efficient finite element formulations for the analyses of strain gradient nanobeams and nanoplates. The present work deals with the investigation of the static, stability and dynamic characteristics of nanobeams and nanoplates undergoing infinitesimal/finite deformation using the second-order strain gradient nonlocal theories.

The governing equations and the corresponding boundary conditions are derived for linear elastic isotropic Euler-Bernoulli beam with second-order positive and negative strain gradients based on Hamilton's principle. The variational statement with C^1 continuity requirement leads to unsymmetric nonlocal terms whereas the symmetrisation of the nonlocal terms leads to C^2 continuity requirement with additional boundary conditions. Analytical solutions for static bending, buckling and free vibration analyses are also derived to validate the finite element models. Results from the C^2 continuous model are found to be in excellent agreement with those from the analytical study. The second-order strain gradient model with negative nonlocal coefficient predicts physically meaningful results matching with the experimental investigations.

The governing equation and the corresponding classical/non-classical boundary conditions are derived for linear elastic isotropic Kirchhoff plate with second-order negative strain gradient term based on Hamilton's principle. Levy's analytical solution approach is extended for the analysis of static bending of rectangular strain gradient plates with different boundary conditions at the edges using the method of superposition. The weak form of the governing equation of motion requires C^2 continuity of transverse displacement. In the present work, a new computationally efficient 4-noded nonconforming rectangular finite element formulation with 6 degrees of freedom per node is presented. From static bending, buckling and free vibration analyses, this element is found to be computationally more efficient with better accuracy and convergence rate than the 4-noded C^2 continuous conforming element with 9 degrees of freedom per node.

The governing equation and the corresponding classical/non-classical boundary conditions are derived for geometrically nonlinear elastic isotropic Kirchhoff plate with second-order negative strain gradient term based on the principle of virtual work. The weak form requires C^1 continuity of the in-plane displacements and C^2 continuity of the transverse displacement. In the present work, a new computationally efficient 4-noded subparametric nonconforming finite element of arbitrary quadrilateral shape with 12 degrees of freedom per node is presented. The performance of the developed finite element is investigated for static bending of rectangular nanoplates involving five different combinations of clamped, simply supported and free edge boundary conditions.

From the detailed investigation, the effects of the positive and negative strain gradient terms are found to be of softening and hardening nature, respectively. Structures with geometry comparable to the microstructural length scale show significant size effect and this size dependency diminishes with the increase in the size of the structure.

सारांश

सूक्ष्म/अतिसूक्ष्म पैमाने पर आकार के प्रभावों को मापने के लिए संशोधित सातत्य सिद्धांतों की आवश्यकता होती है, जो कि किसी भी आंतरिक लंबाई पैमाने के मापदण्ड की अनुपस्थिति में पारम्परिक सातत्य सिद्धांतों के द्वारा संभव नहीं है। साहित्य समीक्षा से यह निष्कर्ष निकाला गया है कि द्वितीय कोटि के विकृति प्रवणता के सिद्धांतों में केवल एक गैर-स्थानीय मापदण्ड शामिल है और विभिन्न भारण/सीमा स्थितियों के लिए समनुरूप गैर-स्थानीय प्रभाव का प्रतिनिधित्व करने में सक्षम हैं। साहित्य में गैर-स्थानीय धरण/चादरों के लिए विकृति प्रवणता के प्रभाव को शामिल करने वाला विश्लेषणात्मक हल विभिन्न सीमा स्थितियों के साथ उपलब्ध नहीं हैं। इसके अलावा, विकृति प्रवण अतिसूक्ष्म धरण और अतिसूक्ष्म चादरों के विश्लेषण के लिए अभिकलनात्मक रूप से कुशल परिमित अल्पांश पद्धतियों को विकसित करने की आवश्यकता है। वर्तमान कार्य द्वितीय कोटि के विकृति प्रवणता के गैर-स्थानीय सिद्धांतों का उपयोग करते हुए बहुत छोटा/परिमित विस्थापन से गुजरने वाले अतिसूक्ष्म धरण और अतिसूक्ष्म चादरों की स्थैतिक, स्थिरता और गतिशील विशेषताओं की जांच से संबंधित है।

द्वितीय कोटि के सकारात्मक और नकारात्मक विकृति प्रवणता के साथ रैखिक लोचदार समानुवर्ती ओइलर-बर्नौली धरण के लिए हैमिल्टन के सिद्धांत पर आधारित संचालन समीकरण और संबंधित सीमा स्थितियां व्युत्पन्न की गयी हैं। सी-१ निरंतरता के आवश्यकता के साथ वाले विवरण कथन में असममित गैर-स्थानीय पद आते हैं जबकि गैर-स्थानीय पदों का सममितिकरण अतिरिक्त सीमा स्थितियों के साथ सी-२ निरंतरता की आवश्यकता की ओर ले जाता है। परिमित अल्पांश प्रतिरूप के प्रमाणीकरण के लिए स्थिर वक्रण, अस्थिरता और मुक्त कंपन विश्लेषण के विश्लेषणात्मक हल भी व्युत्पन्न किए गए हैं। सी-२ निरंतरता वाले परिमित अल्पांश प्रतिरूप के आकलन विश्लेषणात्मक हल के आकलन के साथ उत्कृष्ट समझौते में पाये गए हैं। नकारात्मक गैर-स्थानीय गुणांक के साथ द्वितीय कोटि का विकृति प्रवणता प्रतिरूप प्रयोगात्मक आकलनो के अनुरूप भौतिक रूप से सार्थक परिणाम देता है।

द्वितीय कोटि के नकारात्मक विकृति प्रवणता के साथ रैखिक लोचदार समानुवर्ती किरचॉफ चादर के लिए हैमिल्टन के सिद्धांत पर आधारित संचालन समीकरण और संबंधित पारम्परिक/गैर-पारम्परिक सीमा स्थितियां व्युत्पन्न की गयी हैं। अध्यारोपण के सिद्धांत का उपयोग करके किनारों पर विभिन्न सीमा स्थितियों के साथ आयताकार विकृति प्रवण चादरों के स्थिर वक्रण के विश्लेषण के लिए लेवी के विश्लेषणात्मक हल पद्धति को विस्तृत किया गया है। गति के संचालन समीकरण के शिथिल विवरण कथन में अनुप्रस्थ विस्थापन की सी-२ निरंतरता की आवश्यकता पायी गयी है। वर्तमान कार्य में, एक नये अभिकलनात्मक रूप से कुशल ४-आसंधि वाले गैर-अनुरूपित आयताकार परिमित अल्पांश का सूत्रीकरण ६ स्वतंत्रता चर प्रति आसंधि के साथ प्रस्तुत किया गया है। स्थिर वक्रण, अस्थिरता और मुक्त कंपन विश्लेषण के लिये यह अल्पांश बेहतर सटीकता और अभिसरण दर के साथ ९ स्वतंत्रता चर प्रति आसंधि वाले ४-आसंधि सी-२ निरंतर अनुरूप आयताकार अल्पांश की तुलना में अभिकलनात्मक रूप से अधिक कुशल पाया गया है।

द्वितीय कोटि के नकारात्मक विकृति प्रवणता के साथ ज्यामितीय रूप से अरेखीय लोचदार समानुवर्ती किरचॉफ चादर के लिए आभासी कार्य के सिद्धांत पर आधारित संचालन समीकरण और संबंधित पारम्परिक/गैर-पारम्परिक सीमा स्थितियां व्युत्पन्न की गयी हैं। शिथिल विवरण कथन में अनुदैर्ध्य विस्थापन की सी-१ निरंतरता और अनुप्रस्थ विस्थापन की सी-२ निरंतरता की आवश्यकता पायी गयी है। वर्तमान कार्य में, १२ स्वतंत्रता चर प्रति आसंधि वाले स्वेच्छित ढंग से चतुर्भुज के आकार के एक नये अभिकलनात्मक रूप से कुशल ४-आसंधि वाले उप-प्राचलिक गैर-अनुरूपित परिमित अल्पांश प्रस्तुत किया गया है। विकसित परिमित अल्पांश के प्रदर्शन की जांच आयताकार अतिसूक्ष्म चादरों के स्थिर वक्रण के लिए किया गया है, जिसमें पांच अलग-अलग सीमा स्थितियों के संयोजनों को शामिल किया गया है।

विस्तृत जांच से, सकारात्मक और नकारात्मक विकृति प्रवणता के प्रभाव क्रमशः नरम और सख्त प्रकृति के पाये गए हैं। सूक्ष्म संरचनात्मक लंबाई के पैमाने के साथ तुलनीय आकार की संरचनाएं महत्वपूर्ण आकार प्रभाव दिखाती हैं और संरचना के आकार में वृद्धि के साथ यह आकार निर्भरता कम हो जाती है।

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Nomenclature and Abbreviations

English Notations

a, b	:	Dimensions of rectangular plate along *x*- and *y*-directions
a_e, b_e		Dimensions of rectangular element along *x*- and *y*-directions
a_0	:	Internal characteristic length
A, I	:	Area and second moment of area of beam cross section
$\tilde{A}$	:	Extensional rigidity
$\mathbf{B}_e$, $\mathbf{B}$	:	Elemental and global load vector due to the boundary integral terms
C_{ijkl}	:	Classical stiffness tensor
$\mathbf{d}_i$, $\mathbf{d}$	:	Nodal and global degrees of freedom vectors
$\mathbf{d}_e$, $\tilde{\mathbf{d}}_e$	:	Elemental degrees of freedom vector
$\mathbf{d}_{u_0}$, $\mathbf{d}_{v_0}$, $\mathbf{d}_w$	:	Elemental degrees of freedom vectors corresponding to u_0, v_0 and w
$\mathbf{d}_{u_0 i}$, $\mathbf{d}_{v_0 i}$, $\mathbf{d}_{wi}$	:	Nodal degrees of freedom vectors corresponding to u_0, v_0 and w
$\boldsymbol{\delta}_{u_0}$, $\boldsymbol{\delta}_{v_0}$, $\boldsymbol{\delta}_w$	:	Elemental degrees of freedom vectors corresponding to u_0, v_0 and w involving derivatives with respect to natural coordinates
$\boldsymbol{\delta}_{u_0 i}$, $\boldsymbol{\delta}_{v_0 i}$, $\boldsymbol{\delta}_{wi}$	:	Nodal degrees of freedom vectors corresponding to u_0, v_0 and w involving derivatives with respect to natural coordinates
D	:	Diameter of the beam
$\tilde{D}$	:	Bending rigidity
E	:	Young's modulus
e_0	:	Material constant
e_{ijk}	:	Alternate tensor

f	:	Uniformly distributed axial load
F	:	Transverse point load at the center
$\mathbf{F}_e$, $\mathbf{F}$	:	Elemental and global load vectors
h	:	Thickness along z direction
$\mathbf{H}$, $\tilde{\mathbf{H}}$, $\mathbf{H}_w$	:	Shape functions for w
$\mathbf{H}_{u_0}$, $\mathbf{H}_{v_0}$	:	Shape functions for u_0 and v_0
$\bar{\mathbf{H}}_{u_0}$, $\bar{\mathbf{H}}_{v_0}$, $\bar{\mathbf{H}}_w$	:	Shape functions for u_0, v_0 and w in natural coordinate space
I_0, I_0	:	Translatory and rotary inertia
$\mathbf{J}_1$, $\mathbf{J}_2$, $\mathbf{J}_3$	:	First-, second- and third-order Jacobian transformation matrices
k	:	Wave number
$\mathbf{K}_e$, $\mathbf{K}$	:	Elemental and global stiffness matrices
$\mathbf{K}_{G_e}$, $\mathbf{K}_G$	:	Elemental and global geometric stiffness matrices
l, l_0, l_1, l_2	:	Nonlocal parameters
l_m	:	Inertia related nonlocal parameter
L	:	Length of the beam
L_0	:	External characteristic length
L_e	:	Length of beam element
$\mathbf{M}_e$, $\mathbf{M}$	:	Elemental and global mass matrices
M_{xx}, M_{yy}, M_{xy}	:	Moment resultants about positive y- and negative x-axes, and twisting moment resultant about negative x-axis
n, s	:	Normal and tangential directions
$\mathbf{N}$	:	Shape functions for u_0
N_{xx}, P_{xx}	:	Boundary normal stress resultant and higher-order normal stress resultant on x-face
$\hat{N}_{xx}$, $\hat{P}_{xx}$	:	Specified normal stress resultant and higher-order normal stress resultant on x-face
N_{xy}, P_{xy}	:	Boundary shear stress resultant and higher-order shear stress resultant on x-face

$\hat{N}_{xy}$, $\hat{P}_{xy}$	:	Specified shear stress resultant and higher-order shear stress resultant on x-face
N_{yx}, P_{yx}	:	Boundary shear stress resultant and higher-order shear stress resultant on y-face
$\hat{N}_{yx}$, $\hat{P}_{yx}$	:	Specified shear stress resultant and higher-order shear stress resultant on y-face
N_{yy}, P_{yy}	:	Boundary normal stress resultant and higher-order normal stress resultant on y-face
$\hat{N}_{yy}$, $\hat{P}_{yy}$	:	Specified normal stress resultant and higher-order normal stress resultant on y-face
P_c	:	Critical buckling load
$\bar{P}_c$	:	Nondimensional critical buckling load
$\tilde{P}_{xx}$, $\tilde{P}_{yy}$, $\tilde{P}_{xy}$	:	Applied in-plane compressive forces per unit length along x- and y-axes and applied in-plane shear force per unit length
q	:	Uniformly distributed transverse load
Q	:	Transverse tip load
r	:	Discrete particle radius
$\mathbf{R}_e$, $\mathbf{R}$		Elemental and global internal load vectors
S_{xx}	:	Nondimensional stress distribution
$\mathbf{T}_e$, $\mathbf{T}$	:	Elemental and global tangent stiffness matrices
T_{ij}	:	Classical stress tensor
u, v, w	:	Displacements along x-, y- and z-directions
u_0, v_0	:	Mid-plane displacements along x- and y-directions
$\hat{u}_0$, $\hat{v}_0$, $\hat{w}$	:	Mid-plane displacements along x- and y-directions and transverse displacement specified at the boundaries
U	:	Strain energy
V	:	Volume occupied by the structure
V_{xz}, $\tilde{M}_{xx}$, Q_{xx}	:	Boundary transverse shear stress resultant on x-face, moment resultant about y-axis and higher-order moment resultant about y-axis

$\hat{V}_{xz}$, $\hat{M}_{xx}$, $\hat{Q}_{xx}$	:	Specified transverse shear stress resultant on *x*-face, moment resultant about *y*-axis and higher-order moment resultant about *y*-axis at $x = \pm a/2$
V_{yz}, $\tilde{M}_{yy}$, Q_{yy}	:	Boundary transverse shear stress resultant on *y*-face, moment resultant about *x*-axis and higher-order moment resultant about *x*-axis
$\hat{V}_{yz}$, $\hat{M}_{yy}$, $\hat{Q}_{yy}$	:	Specified transverse shear stress resultant on *y*-face, moment resultant about *x*-axis and higher-order moment resultant about *x*-axis at $y = \pm b/2$
$\bar{w}$	:	Nondimensional transverse displacement
w_c, w_p	:	Homogeneous solution and the particular integral
w_{nl}, w_l	:	Transverse displacements with and without nonlocal effect
x, y, z	:	Cartesian coordinates
x_e, y_e	:	Local element coordinates in physical coordinate space

Greek Notations

α	:	Nonlocal kernel
χ_{ij}^{s}	:	Symmetric rotation gradient tensor
δ_{ij}	:	Kronecker delta tensor
Δ	:	Percentage reduction in central/maximum transverse displacement
ε_{kl}	:	Classical strain tensor
ε_{xx}, ε_{yy}, γ_{xy}	:	Normal strains in *x*- and *y*-directions and in-plane shear strain
ε_{xx}^{0}	:	Extensional strain
$\hat{\varepsilon}_{xx}$, $\hat{\gamma}_{xy}$	:	Normal strain and shear strain specified at $x = \pm a/2$
$\hat{\varepsilon}_{yy}$, $\hat{\gamma}_{yx}$	:	Normal strain and shear strain specified at $y = \pm b/2$
Γ	:	Boundary surrounding the structure
γ_i	:	Dilatation gradient vector
$\eta_{ijk}^{(1)}$	:	Deviatoric stretch gradient tensor

κ_{xx}	:	Bending curvature
λ , μ	:	Lamé constants
υ	:	Poisson's ratio
$\hat{\theta}$, $\hat{\varepsilon}_0$, $\hat{\chi}$	:	Slope, axial strain and curvature specified at the boundaries
$\hat{\theta}_x$, $\hat{\chi}_x$	:	Slope about *y*-axis and curvature along *x*-axis specified at the boundaries $x = \pm a/2$
$\hat{\theta}_y$, $\hat{\chi}_y$	:	Slope about *x*-axis and curvature along *y*-axis specified at the boundaries $y = \pm b/2$
ρ	:	Mass density
σ_{ij}	:	Nonlocal stress tensor
σ_{xx} , σ_{yy} , τ_{xy}	:	Normal stresses in *x* and *y* directions and in-plane shear stress
ω	:	Fundamental natural frequency
$\bar{\omega}$	:	Nondimensional fundamental natural frequency
ω_m	:	Natural frequency of the m^{th} mode
$\bar{\omega}_m$	:	Nondimensional natural frequency of the m^{th} mode
Ω	:	Surface area occupied by the structure
ξ , η	:	Natural coordinates
ψ	:	Compression ratio
∇^2	:	Laplacian operator

Abbreviations/Acronyms

AFM	:	Atomic Force Microscopy
AIREBO	:	Adaptive Intermolecular Reactive Empirical Bond Order
CC	:	Clamped-clamped
CCCC	:	All edges clamped
CF	:	Clamped-free/Cantilever
CNT	:	Carbon nanotube
CS	:	Clamped-simply supported/Propped cantilever
DLGS	:	Double-layered graphene sheet
DWCNT	:	Double-walled carbon nanotube

FDM	:	Finite Difference Method
FE1	:	Finite Element Formulation with C^1 Continuity
FE2	:	Finite Element Formulation with C^2 Continuity
FEM	:	Finite Element Method
MCST	:	Modified couple stress theory
MD	:	Molecular dynamics
MEMS	:	Micro-electro-mechanical systems
MLGS	:	Multi-layered graphene sheet
MSGT	:	Modified strain gradient theory
MWCNT	:	Multi-walled carbon nanotube
NEMS	:	Nano-electro-mechanical systems
SCSC	:	One pair of non-adjacent edges simply supported and the other pair clamped
SCSF	:	One pair of non-adjacent edges simply supported while the third edge clamped and the fourth edge free
SFSF	:	One pair of non-adjacent edges simply supported and the other pair free
SLGS	:	Single-layered graphene sheet
SS	:	Both ends simply supported
SSSS	:	All edges simply supported
SWCNT	:	Single-walled carbon nanotube
UDL	:	Uniformly distributed load