Chapter

Finite Element Analysis in Nanotechnology Research

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Abstract

The Finite Element Analysis in the field of Nanotechnology is continually contributing to the areas ranging from electronics, micro computing, material science, quantum science, engineering, biotechnology, medicine, aerospace, and environment and in computational nanotechnology. The finite element method (FEM) is widely used for solving problems of traditional fields of engineering and Nano research where experimental analysis is unaffordable. This numerical technique can provide accurate solution to complex engineering problems. Over decades this method has become the noted research area for the mathematicians. The popularity of FEM is due to the advent of computer FEA software such as NASTRAN, ANSYS, ABAQUS, Matlab, OPEN Foam, Simscale and the like. With the development of nanoscience, the researchers found difficulties in spending funds for nano related projects. The FEA has evolved as the affordable methodology and offers solutions to all complicated systems of research.

Keywords: nanotechnology, FEM, FEA, research, nanoscience

1. Introduction

"To move precisely in nanoworld, you donot succeed by perfecting proven techniques".- Handelsblat. [1] . As stated, the nano research requires newer methodologies and techniques to be worked out to succeed. The microtechnology to nanotechnology needs a factor of thousand for size reduction. Different methodologies exist to club cooperation between macro, micro and nano robots and analytical based FEM for static, modal, harmonic and transient analysis of structures. Clubbed with multiparametric optimization and neural networks, FEM had developed as an optimal solution to all complicated problems of engineering, science, technology, medicine and research. The "bottom up" technology of late twentieth century promises the use of robotics for micro/nano manipulation processing [1]. The revolution of computers had led to development of closed form solutions which are extremely difficult to be obtained for any engineering problems [2]. This urge leads to adopting any one of the numerical techniques. FEA had been one of the options of researchers and choice of the method depends on the familiarity of the users. FEM exploits the research methodologies using direct approach, variational approach, direct approach, energy approach, weighted residual approach, Isoparametric formulation, static condensation and nonlinear analysis [2]. Numerical approximations can be reached by differential equations and PDE for various mathematical and nano technology problems of applied physics. FEM explores checking the validity of analytical studies of nanotechnology. Moreover the unaffordable experimental setup of nanoresearch could be replaced with FEA software as observed by engineers and scientists working on the field [2].

2. Applications of FEM in nano research

2.1 Electrospun nanofibrous Mats under biaxial tension

The nanofibrous mats can be used as freestanding electrodes in energy storage devices. These mats have non uniform material properties [3] with each and every single fiber having nonlinear characteristics. The research came up with two macroscopic continuum models with uniform or oriented nanofibre distribution to exactly replicate the nanofibrous mats under biaxial tension. The mechanical response of electrospun SF/PCL nanofibrous mats was explored. The model simulated by FEM exposed the deformation of nanofibrous mats and the gradual damage mechanism along with the microstructure.

2.2 Carbon nanotube reinforced composite's stress transfer

The improvement [4] in mechanical properties of hybrid composite system strongly depends on interfacial mechanical properties (interfacial stress transfer efficiency). The interfaces are zones of structural, compositional and property gradients. The width varies from single atom to micrometers. The properties of the composite depend on the surface of the single fiber and the resin used for bonding. The stress transfer of SWNT reinforced composite was studied using hybrid FEM approach. Three dimensional REV (representative elementary volume method) had been used along with Molecular Dynamics (MD) to exploit the stress transfer mechanism of CNT reinforced composite. The [4] effects of fiber volume fraction, interfacial stiffness and elastic modulus on the stress of the matrix were explored. The analytical models are difficult along with experiments in nanoscale as they are too expensive. Hence FEM simulated models were used to predict the stress transfer and found to be accurate on validation.

2.3 Formulation of 3D finite element implementation for adhesive contact at nanoscale

A research was carried out [5] for three dimensional nanoscale contact problems with strong adhesion. The contact description was based on Lennard Jonnes [5] description suitable to explain Vanderwaals attraction between interacting bodies. By incorporating the potential into nonlinear continuum mechanics, formulations had been arrived for surface force and body force. Based on these formulations, overall contact algorithm had been arrived using FEM. This model has an application in biomechanics as denoted by adhesion of gecko spatula [5]. Efficient FE formulation was arrived based on surface traction. The behavior of contact model described by SF formulation was more efficient than BF formulation for strong adhesive existence.

2.4 Finite element simulation of micromachining of nanosized silicon: carbide particle reinforced composite

The nanosized silicon – carbide – particle (SICp) reinforced aluminum matrix composite's micromachining process had been studied [6] using finite element method. The parameters of cohesive zone model had been found from stress – displacement curves of the molecular dynamics (MD) simulation. The model represented exactly the random properties of silicon – carbide particle distribution and the interfacial bonding between SICp and matrix [6]. The mechanism of machining was analyzed as per chip morphology, stress variation, temperature and cutting force. The FE simulation projected the fact that SICp caused non uniform interaction between the tool and reinforcement. The deformation mechanics [6] led to inhomogeneous stress variation and irregular cutting force.

2.5 FE modeling of double walled CNT based sensor

The Carbon Nanotubes (CNTs) are widely used for designing nano sensors, nano resonators and actuators [7]. The mass sensing characteristics of defective Double Walled Carbon nanotubes (DWNTs) were studied using FEM. Various finite element simulations covering chiral, zigzag and arm chair nanotubes with cantilever and bridged conditions using molecular [7] structural dynamics approach. The defects have been subdivided in to 6 missing atoms (A type) and 24 (B type) missing atoms on the outer wall of DWNT. COMBIN 14 element had been used for simulation of defective DWNTs with weak Vanderwaals force. The study revealed the fact that the frequency of defective DWNT reduced with increase in chiral angle. Also the frequency reduced with increase in pinhole defects.

2.6 Perspective on nanotips

Numerous methods have been fabricated for developing ultra-sharp tips for scanning probe microscopy and [8] electron microscopy. It has been observed that the sharp end terminates with very single atom in field ion microscope (FIM). The last atom had been intended to form atomic channel of electrons in field emission mode which would self-collimate a coherent electron beam with an outstanding brightness. Hence nanotips are found to behave as a source of self-collimated electron or ion beam. In this research [8] the distribution of electric field in the vicinity of nanotip apex that holds the topmost single atom had been studied analytically and numerically. The tip base was found to dominate nano protrusions which enhance electric field. The study revealed that nanotips with broad bases produce even less field than modest tips at the same voltage. This pronounced the fact that the tip base accounts for high voltages needed at imaging threshold field.

2.7 Axial vibration of embedded love – Bishop nanorods

In this research, nonlocal free vibration of axial rods embedded in elastic medium had been studied using Love – Bishop rod theory with FEM. Constitutive modeling for rod formulation using kinematic relations and dynamic equilibrium had been analyzed. Equation [9] of motion and boundary conditions were obtained by varying total potential of nano rod and were solved using separation of variation. Frequency equations of 4 types of nanorods were obtained. Size dependent FEM formulation was synthesized based on weighted residual method. The four parameters mode number, non-local parameter, rod length, and slenderness ratio were used to study the frequency parameters of nanorods. The free vibration frequencies of the simple axial rods had been found to be higher than that of Love bishop rods. These were evaluated by frequencies of two rod theories in higher modes.

2.8 Bending analysis of embedded nano plates using FEM

Eringen's nonlocal elasticity theory is capable to capture small length scale effect. Hence it is widely used to explore the mechanical behavior of nanostructures [10]. Instead of using differential form, the integral form should be used to avoid inconsistency in results. Arbitrary kernel functions are used for general form. The first order [10] shear deformation theory is used to model the nanoplates. The study evaluates the first order shear deformable embedded nanoplates for bending using Erignen's nonlocal theory. Using FEM approach the maximum deflection of the structure was evaluated. The results pronounced that the clamped or simply supported boundary conditions provided same trend for the effects of non-local parameter on the bending analysis of nano plate for Erignen's integral and differential formulation. Also the results proved that the elastic foundation increased the stiffness of the structure and decreased the influence 0f nonlocal parameter.

2.9 Stresses at bone: particle reinforced nano composite interface

The biomaterial should satisfy its bio functionality and biocompatibility. The tissue – implant interface plays a huge role in both the parameters. Nanobioceramics is a newer technology that had widened [11] range of biomedical and dental applications including increased bioactivity for tissue regeneration and engineering, drug and gene delivery, treatment of viral infections and implantable surface modified medical devices for [11] better hard and soft tissue attachments. FEA had been accepted for simulations in biomechanics for analyzing stresses and strains in dental implants and surrounding bone structures. The tissue engineering needs combining 3D scaffolds with living cells to deliver the much needed cells to damage sites in the human body. This scaffold should be capable of making cells to attach and multiply. Hence the design of scaffold is a challenging task which could be narrated by the finite element analysis. Also the nanotechnology had revolutionized nanobiomaterials, tissue engineering nano scaffold, nano – drug delivery and dental nanocomposites [11].

2.10 Elastic plastic analysis of ultrafine grained Si2N2O – Si3N4 composites

The development of micro/nanotechnology [12] had led to characterization of the mechanical properties at micro- and nano- scales. The nano indentation test has a diamond indenter to produce indentation load and the penetration depth from which load – penetration curve (P-h) is obtained. The P-h curve can be used to define mechanical properties including hardness, elastic modulus and toughness [12]. Only few studies had been reported on elastic–plastic property of brittle bulk ceramics. There are two methods to derive material properties from loading and unloading indentation curves. One of the curves involves the use of unloading curves and classical elastic solution of infinite half space [12]. This method is suitable for calculating the hardness and elastic modulus of materials. Another methodology involves producing loading and unloading response curves for various parameters through finite element modeling. Stress strain relations can be produced by using the nanoindentation experiment. The ultra-fine – grained Si2 N2O – Si3N4 had been produced by hot press sintering of amorphous nano – sized silicon nitride powders at 1600, 1650 and 1700 Deg Celsius with nanosized additives. After evaluating by nano identation through finite element formulation, the elastic modulus and P-h curve are obtained. A newer theoretical methodology for evaluating stress strain relation of brittle ceramic materials had been identified. Numerous coefficients in theoretical calculation formula had been found using calculation and simulation results.

2.11 Torsional statics and dynamics of circular nanostructures

Newer technologies for developing advanced materials [13] and structures are advancing towards a minute length scale (i.1., micro – or nano – scale). This is the root of nanotechnology. By reducing the size of the materials, the materials exhibit specific and interesting non classical mechanical, chemical and electrical properties. The classical continuum theories fail to replicate the minute length scale [13]. Hence explicitly new continuum mechanics /atomic dynamic simulation are required. Erignen developed Non local elasticity theory as one of the continuum models. In this research, the torsional static and dynamic nonlocal effects for circular nanostructures for concentrated and distributed torques were investigated based on nonlocal elasticity stress theory [13]. Variational energy principle is obtained to derive governing differential equation and strain energy and kinetic energy components are obtained. A new nonlocal finite element method (NL-FEM) had been developed to solve integral nonlocal equation. The statics and dynamics of nonlocal nanoshafts, nanorods, and nanotubes with various loads and boundary conditions revealed possible numerical solutions which were compared with analytical solutions.

2.12 Elastic properties of coiled CNT reinforced Nano composite

With the invention of Carbon nanotube with advanced material properties, various nano composites had been developed [14]. A new algorithmic representative volume element (RVE) and finite element method had been formulated to find the elastic properties of coiled Carbon NanoTubes (CCNT). The elastic properties had been explored with the respect to interphase, fiber volume fraction, orientation, number of coils, tube diameter, coil diameter and helix angle using FEM. The elastic moduli of the nanocomposites were found to decrease with increase in the number of coils. Also it had been found that SWNT offers better reinforcement when compared with CCNT reinforcement.

2.13 Elastic and fracture characteristics of graphene – silicon nanosheet composites

Graphene and its composites find application in various fields of aerospace, bioelectric sensors, bio engineering, electronics, energy technology, and lithium batteries due to appreciable electrical, mechanical and thermal properties. The single layer graphene sheets (SLG) needs an appropriate substrate which should not alter the properties of graphene. In this research, an efficient method was developed for evaluating nonlinear stress strain behavior and fracture strength of graphene – silicon nanosheet composites. Nonlinear finite element model [15] had been evolved to obtain constitutive model of the problem which are computed using molecular dynamics (MD) simulations. Graphene is modeled as multilinear elastic and silicon is simulated as isotropic material. Using this model nonlinear behavior of graphene, silicon and their stress strain curve including inflection point leading to failure had been arrived. The results of stress strain curves and elastic modulus and the critical stress of single layer graphene (SLG), silicon nanosheet and their composites with different thickness of silicon nanosheet agrees with that of the molecular dynamics [15].

2.14 Thermo electric bulk and nanostructured materials

Numerous analytical solutions had been formulated [16] for coupled nonlinear behavior of thermoelectric device in one dimension. These devices are used in refrigeration and energy harvesting. In this research, a nonlinear model of thermoelectricity was developed using finite element method. The simulated model takes in to account Seebeck, Peltier and Thomson effects [16]. The FEM is represented in potential variables i.e., voltage and temperature and solved using Newton method by formulating stiffness and Jacobian matrices. The results were verified with simulated one dimensional model. The FEM is then implemented to estimate energy conversion of nanostructured thermoelectric materials. Thus the advantages of nanostructured materials lie in the increased performance and miniaturization.

2.15 FEM of nano: indentation to characterize thin film coatings

Thin film coatings [17] are used in tribological, corrosion resistance of mechanical components, tooling, biomedical implants, electronics, microsystem packaging, cutting tool coatings and magnetic devices. The film coatings are explicitly used for reducing wear and tear. It is a current need to investigate the thin film coatings for critical loads that lead to ultimate fracture. Since nanoindentation is a nondestructive one, it is preferred and imperatively it could be simulated by finite element method (FEM). Using FEM, the hardness, elastic modulus, endurance loads, optimal thickness, optimal critical load, stress distribution and contact pressure between substrate and layer could be found.

2.16 Electric field gradients and bipolar electrochemistry effects

The effects of electric field in alternating (AC) and direct (DC)voltages had been explored in vivo and vitro with [18] electrodes in connection with tissues and implanted cells. The electro simulation through noncontact wireless settings by dipoles by bipolar chemistry is highly possible. FEM studies with same configuration that of experimental studies had proved that the voltage profiles are in qualitative agreement with known bipolar effects. There exist [18] a clear mapping of charge gradients at the material surface leading to growth of neurons. The insulating materials distort the electric space distribution while the dipole at the border of implanted conducting material extends along the material surface and much smoother in intercalation materials.

2.17 Elastic stability of curved nanobeam by finite element approach

The elastic stability of curved nanobeam had been investigated using Eringen's strain driven model [19] coupled with higher order shear deformation theory. The influence of different structural theories and analyses of nanobeam is taken into account while deducing the model. The governing differential equation is solved by finite element method using 3 –noded curved beam. The model had been validated using analytical/numerical solutions. The parameters such as thickness ratio, beam length, rise of curved beam, boundary conditions and size dependent [19] or nonlocal are analyzed based on buckling behavior of curved nanobeams. The results prove that the type of buckling mode corresponding to lowest critical value would be varying based on geometrical and internal material length scale parameter and boundary conditions [19].

2.18 Tensile modulus of CNT reinforced polypropylene composite

The reinforcing efficiency of carbon nanotubes (CNTs) in polymers had been found using finite element modeling. The probability distribution functions [20] of CNT diameter, orientation, dispersion and waviness had been incorporated in the finite element model to derive how the CNT characteristics affect the tensile modulus of CNT reinforced polypropylene composite. The scanning electron microscopy images of CNT/PP composites made by melt mixing and injection molding had been used by image analysis approach [20]. The predicted model had been found to be experimentally correct as per ASTM D638.

3. Conclusion

The FE methods had been used to study thermo-electrical–mechanical coupled model. The integrity of lumped element, distributed element and system level element for design, modeling and simulation of nano/micro mechanical systems (N/MEMS) had been achieved by FEM. The nanostructures, nanocomposites and CNTs and their composites had been modeled using FEA. Further FEM had been applied in nanomaterials and systems used in medicine, dental science, biotechnology and electric field in the form of electrospinning.

The investigation of material properties with 1 – 100 nm dimensions had been achieved by nanoscience and technology. Thanks to nanotechnology and FEM, one of the dimensional materials such as CNTs, silica carbide nanotube, nanowire, nanorod and nanobeam had been dream of innovation. The field effective transistors, gas sensors, nanoactuators, nanocantilevers are the live examples. It has been found that these structures have varied applications in nano/micro – electro – mechanical systems (NEMS /MEMS). Ultra capacitors had been found application in hybrid cars. This chapter elaborated the applications of finite element method in varied applications of nanotechnology including CNTs, nano beams, nanorods, nanobiomaterials, graphene coated materials, nanosensors, nanotips and curved nanobeams. Apart from these applications the nanotechnology extends hands to day to day applications such as self-cleansing walls, wall claddings, reinforcement to cement matrix. The FEM could be extended to these materials which had not been extensively covered. A correct mechanical model simulated by finite element modeling would replicate the exact experimental setup and provide solutions to constitutive modeling and all engineering problems. The best example is the usage of CNTs as reinforcements in composites and cementitious materials. The CNTs are costlier that almost 85% of the CNT reinforcement is studies using FEA software by the researchers instead of experimental studies. The last few decades had been dedicated to CNTs, sensors, diagnostic probes and multifunctional materials based on CNTs, electronic devices and energy storage devices. The sensors could be used to monitor all kind of structures including cracks in bridges and structural collapses of civil engineering structures. The replacement of silicon based sensors and transistors with CNT based printed transistors are future challenge and already researches are on using FEM and FEA software. With advent of computers and FEA software such as ANSYS, ABAQUS, NASTRAN the unaffordable experimental analysis of nanoscience had been replaced with analytical studies using FEM.

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