Techniques for Computational Modelling and Analysis of Nanocomposite: A Review

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Abstract: The nanomaterials era has attracted the structural scientists, engineers and industries with basic focus to structure and grow new multifunctional nanocomposite materials with one of a kind blend of properties unattainable with conventional materials. In this paper discussed about modeling methods of nanocomposite and evaluation of material properties. Also discussed the various case studies conducted by different researchers.

***Index Terms* - Nano technology, Nanocomposite, Carbon Nanotube(CNTs), modeling technique, finite element modeling,**

I. Introduction

Nanotechnology, short Name "Nanotech", is the study of the control of matter on an atomic and molecular scale. Generally, nanotechnology deals with structures of the size 100 nanometers or smaller, and involves developing materials or devices within that size. The prefix "Nano" stems from the ancient Greek for "dwarf". In science, it means one-billionth (10-9) of something, thus a nanometer (nm) is one 0.000000001 meters [1]

1. 1 Composite:

Composites are a combination of two materials in which one of the material is called the reinforcing phase, is in the form of fibers, sheets, or particles, and is embedded in the other material called the matrix phase. Fibers or particles embedded in matrix of another material are the best example of modern-day composite materials, which are mostly structural [2].

1.2 Nanocomposite:

The nanocomposite is composed of continuous matrix and discontinuous reinforcement phase. There are three types of material: polymer, ceramic and metals. Each material is being specific material properties of nanocomposite. Ceramic are very strong, brittle, chemical resistant and insulating. Polymer are used for ductile, impact resistant and insulating [3].

1.3 Carbon Nanotubes

Carbon nanotubes (CNT) were discovered in 1991[4]. A single-walled nanotube (SWNT) is a graphene sheet that is rolled into a cylindrical shape so that the structure is one-dimensional with axial symmetry. The interlayer separate in multi-walled nanotubes(MWNT) is near the separation between graphene layers in graphite The outer diameter of MWNT actually depends on the growth process and typically 6. Horizontal-Horizontal magnetic core drilling machines with angular gears are made for confined drilling situations of order 20nm and up to 100nm [5].CNTs ideal fora wide range of applications, including as advanced filler materials in polymer–matrix composites. CNTs/polymer composite improved electrical and mechanical properties in added 1% fraction of polymer. Mechanical and Electrical properties both dependent of quality of CNT [7].

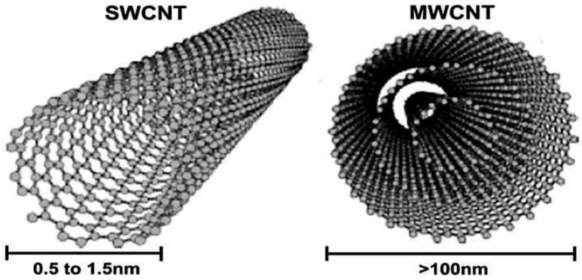

Figure 1: Single-Walled nanotube and multi-walled nanotubes [6].

Hybrid composites contain more than one kind of carbon/fiber in a framework material. On a fundamental level, a few unique fiber types might be consolidated into a half breed, however all things considered, a blend of just two sorts of strands would be generally advantageous. They have been created as an intelligent continuation of traditional composites containing one fiber. Mixture composites have special highlights that can be utilized to meet different plan necessities in a more affordable route than ordinary composites. This is on the grounds that costly filaments like graphite and boron can be incompletely supplanted by more affordable filaments, for example, glass and Kevlar. A portion of the explicit focal points of half breed composites over ordinary composites incorporate adjusted quality and firmness, adjusted twisting and film mechanical properties, adjusted warm bending strength, diminished weight or potentially cost, improved impact resistance improved fracture toughness improved weakness opposition, diminished indent and crack arresting properties, [8].

II. Method And Materials

Computational analysis of composite structure and behavior in case of load application is based on use of numerical integration of the state equations by transforming the system of partial differential equations to a system of linear and linearized algebraic equations with the subsequent solution by means of the mathematical apparatus of the calculus of variations. Nowadays, the finite-element method (FEM) is a commonly used numerical algorithm realized in analytical software applicable for this purpose. The application of FEM as the computational tool is associated with calculation of a significant number of equations and requires high performance computing resources. However, this method is able to perform calculation of samples with complex geometry and structure. The advantages associated with calculations of complex geometry by usage of linear and linearized equations systems are achievable only through realization of function of the sample partition to the nodes and finite-elements. In case of computing software this partition is realized as meshing step [9].

2.1 Voigt upper bound and Reuss lower bound (V-R model):

Voigt upper bound is apply when position of reinforcement material is Aligned and matrix material is a uniform strain direction same to the reinforcement material Voigt got the effective modulus in the reinforcement direction [10].

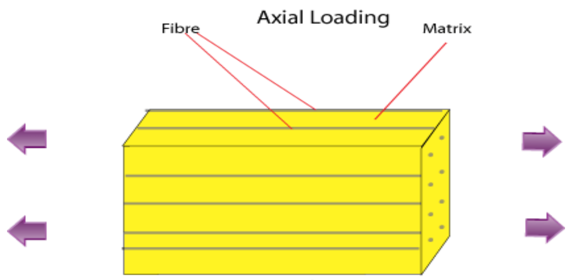

Figure 2: Voigt upper bound (Axial load) [11]

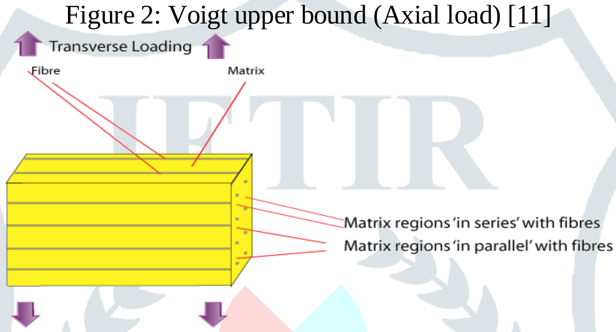

Figure 3: Reuss lower bound (Transverse load) [11]

Reuss applied the same uniform stress on the fiber and matrix in the transverse direction (normal to the fiber direction), and got the effective modulus in the transverse direction [10].

2.2 Halpin -Tsai equation:

Halpin Tsai, empirically developed some generalized equations that readily give satisfactory results compared to the complicated expressions. They are also useful in determining the properties of composites that contain discontinuous or short fibers oriented in the loading direction [12].

The forecast of modulus of a material containing silica Nano particles is displayed by the Halpin-Tsai micromechanical show, which is a notable hypothesis to foresee solidness of composites as an element of filler stacking and perspective proportion [13]. Halpin-Tsai equations are given reliable estimate for the stiffness properties of the nanocomposite and are often applied for comparison with experimental test results [14].

2.3 Analytical micromechanical models:

Analytical micromechanics serve as a quick way to predict the properties of materials and assess the validity of results obtained by numerical simulations. They are, however, insufficient to model the complex microstructures of present-day Nano-composites. The shortcoming is that these methods are highly customized to a specific microstructure, Analytical micromechanical models can be classified into two main categories (1) Rule of Mixtures and (2) Mori– Tanaka. [14]

Rule of Mixtures:

The rule of mixtures is a simple analytical expression to predict the effective material properties for composites. It is based on strength of materials. This concept along with some extended results in the case of fiber reinforced composites has been successfully applied in the past for carbon nanotube based nanocomposites using different RVEs. All the computations are executed on an RVE to carry out the analysis of CNT reinforced nanocomposites. [15].Unidirectional composite may be modeled by assuming reinforcing material to be uniformed in properties and diameter, parallel and continuous throughout the composite. The RVE of this composite is shown in fig 4. It is accepted that ideal holding exists between the fibers and the matrix [16].

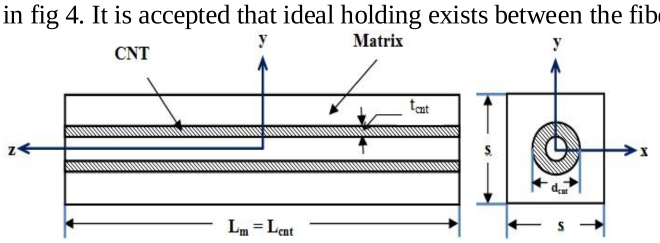

Figure 4: RVE Model of a Matrix and CNT [15]

Mori-Tanaka model

Mori-Tanaka model determine the overall elasticity tensor of the nanocomposite materials. The key suspicion in this model is the average strain in the consideration, that is fiber, is identified with the average strain in the frameworkby a fourth request tensor. This fourth request tensor gives the connection between the uniform strains in the consideration implanted in an all matrix material. Further this material is exposed to uniform resist endlessness. These model describe the effect of basic parameters such as the volume fraction of CNTs within the bulk resin, their statistical orientations, lengths and curvatures [7,17].

2.4. Python based model

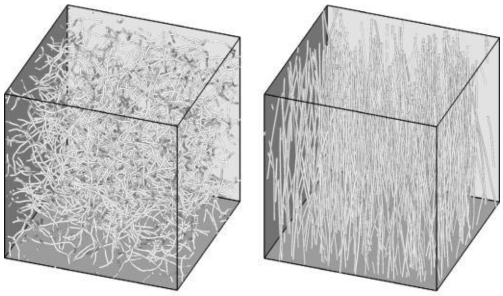

Figure 5: CNT-cables in RVEs: (a) a random distribution and (b) an aligned distribution. [16]

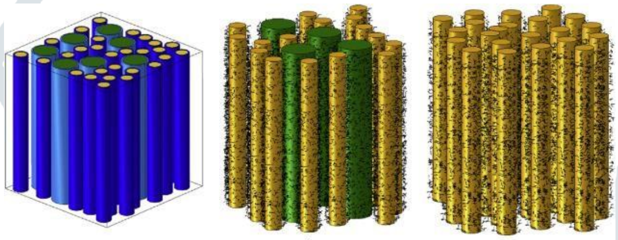

Figure 6: multi element unit cells (a) glass/carbon hybrid composite without CNT (b) with CNT reinforcement, (c) carbon reinforced composite with CNTs [18]

When large difference of the measurement size of the fiber fortified composite and CNTs reinforcement, there is use multiple-step modeling and evolution of material. In this model study of microstructure strength connections of half and half composites with auxiliary CNT reinforcements, various 3D computational models mirroring the hybrid composite structures ought to be created by the Python based software code. A generate code permits to create progressive FE models with predefined structures, including the full scale unit cell and lower scale unit cell show with adjusted/irregular situated carbon nanotubes, encompassed by the effective interface layers, automatically. Examples of the models are shown in fig.6.

Applicability to wind turbine blade materials, It was take three types of material using. (a) glass and carbon composite both are equal (without CNT), (b) with CNT and (c) carbon reinforcement with CNTs.it is used Numerical investigations and decide the weakness lifetime of composites with different structures under perfect dry conditions and expected seaward Service conditions (seawater moistness 65%). Having decided the neighborhood properties of the stages (carbon and glass filaments) under both dry and high dampness Conditions in our computational models and looked at the exhaustion exhibitions of various composite structures. [18]

III. PROPERTY EVOLUTION AND APPLICATIONS

Mechanical: Nanoparticles commonly improve the mechanical properties of polymers, due to the intrinsic characteristics of Nano sized metals such as large surface area and high modulus. The reinforcement effect will be improved by larger and the strong interfacial interactions between filler and matrix. [19,20]

Electrical: The dielectric constant increased with Nano silica loading and reached an optimum at about 10 wt.%. Volume conductivity, dielectric loss factor and dissipation factor [21,22].

Optical: Polymer based inorganic nanocomposite gives good stability and easy process ability with interesting optical properties. The optical properties of nanomaterials depend on parameters such as feature size, shape, surface characteristics, and other variables including doping and interaction with the surrounding environment or other nanostructures. [19,23]

APPLICATION:

Applications of eco-friendly and sustainable Nano reinforced composites are in,

- Automotive (gas tanks, bumpers, interior and exterior panels).
- Construction (building sections and structural panels).
- Aerospace (flame retardant panels and high performance components).
- Electrical and electronics (electrical components and printed circuit boards).
- Packaging (containers and wrapping films).
- Medical Science (Orthopedic, dental, tissue engineering).
- Automation Equipment (Sensors, Actuators). [19]

IV. CONCLUSION

Study conducted on different methods available for modelling of composite material and property evaluation. Modelling Methods used for determine composite fraction, aspect ratio, stiffness of the material and to modify composite is easily. After comparison of different research work, Halpin-tsai models demonstrated an exceptionally decent understanding when contrasted with the tentatively estimated qualities. Analytic functions did not yield more accurate results in comparison to the even analytic polynomial functions.

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