COMPUTATIONAL MATERIALS AT NASA LANGLEY RESEARCH CENTER

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Summary

The paper provides a description on the structure and implementation of the Computational Materials Program at the NASA Langley Research Center. An example is given that illustrates the suggested approaches to predicting the behavior and influencing the design of nanostructured materials such as carbon nanotube-reinforced polymers. Primary simulation and measurement methods applicable to multi-scale modeling are outlined and presented within the context of predicting the global buckling behavior of a carbon nanotube/polymer orthotropic plate with both functionalized and nonfunctionalized nanotubes.

Introduction

Each distinct age in the development of humankind has been associated with advances in materials technology. Within the last 20 years, several research institutions have recognized the need for a more systematic approach to new materials development, i.e. "Computational Materials." This approach is one that would combine interdisciplinary research, new advances in computational modeling and simulation, and critical laboratory experiments to rapidly reduce the time from concept to end product.

Computational Materials at Langley Research Center (LaRC) draws from physics and chemistry, but focuses on constitutive descriptions of materials that are useful in formulating macroscopic models of material performance.[1] The purpose of this paper is to describe in some detail how convergent technologies have facilitated the LaRC Computational Materials approach for aerospace materials and structures research. In particular, the paper discusses how the Computational Materials program at LaRC proposes to utilize multi-scale analysis methods to establish the technology for the scale-up of nanostructured materials into definition at the macro or engineering level for advanced aircraft and spacecraft. Primary simulation and measurement methods applicable to multi-scale modeling are outlined and presented within the context of predicting the global buckling behavior of a carbon nanotube/polymer orthotropic plate with both functionalized and nonfunctionalized nanotubes.

Model Development

In order to address the goals and challenges, the Computational Materials program has developed a scheme for spanning both the length and time scales associated with analyses that describe material behavior. The starting point is at the atomistic scale for initial model development. Models at this scale are based on molecular mechanics or molecular dynamics. At the next scale, the models can incorporate micro-scale features

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and simplified constitutive relationships. Further progress up the scale leads to the meso or in-between levels that rely on combinations of micromechanics and well-established theories such as elasticity. The last step towards engineering-level performance is to move from mechanics of materials to structural mechanics by using methods that rely on empirical data, constitutive models, and fundamental mechanics.

The nanostructured materials based on carbon nanotubes and related carbon structures are of current interest for NASA. To be used as a structural material, single-walled carbon nanotubes (SWNTs) must contribute to the design by providing capabilities to increase structural performance. Buckling resistance is an important consideration in the design of thin-walled, lightweight aerospace vehicle structures. Thus, studies of the effects of SWNT structure on the global buckling resistance of a basic structural element, such as a flat plate, serve as a first-order means for assessing the potential of SWNT-reinforced polymeric composites. As a natural progression toward this type of global assessment, several studies that examine the compressive buckling behavior of an individual nanotube, unsupported by a surrounding matrix, have been conducted using a range of analysis techniques [2], [3], [4]. The typical representation of a SWNT is a cylindrical, lattice structure of carbon atoms with a tube diameter of approximately one nanometer and tube length varying from tens of nanometers to ten of microns.

The emphasis of these previous studies was on selected modes of failure associated with compression loading: nanotube buckling and local stability. The objective of the present paper is to develop a multi-scale analysis model to predict the influence of molecular attributes on the macro-scale, global structural stability of an SWNT-polymer composite plate subjected to a general state of in-plane mechanical loads. The determination of the SWNT-polymer composite elastic stiffness properties used in the current study was described previously by Odegard, et al. [5] In this previous study, the mechanical behavior of the SWNT-polymer composite was assumed to depend not only on the individual properties of the polymer and the nanotubes, but also on the nanotube/polymer interaction. Four molecular-level structural items were defined by this previous study as the primary molecular attributes, controlled at material synthesis, which could influence final properties of the composite. These four attributes were nanotube length, volume fraction, nanotube orientation, and nanotube functionalization. The latter item, nanotube functionalization, was defined as the formation of a chemical covalent bond between the nanotube and polymer directly. The influence of these four intrinsic structure attributes on bulk constitutive properties was investigated using a hierarchical modeling approach. [6], [7]. The material system used in this study was a carbon nanotube reinforced polymer composite. The carbon nanotube material was modeled as a single-walled (10,10) nanotube of radius 6.78 Å and variable length. The polymer matrix material was assumed to be isotropic, amorphous polyethylene matrix

with a representative Young's modulus and Poisson's ratio of 0.9 GPa and 0.3, respectively.

Using a hierarchical modeling scheme, the equivalent-continuum modeling technique of Odegard, et al. was used to predict the bulk elastic properties. Briefly, the hierarchical modeling method relies on three major steps. First, a suitable representative volume element (RVE) of the nano-structured material is chosen based on the geometry of the molecular model where the geometry of the molecular structure was defined by molecular dynamics simulations Second, an equivalent-truss model of the RVE is developed as an intermediate step to link the molecular and equivalent-continuum models. Finally, an equivalent-continuum model of the RVE is developed in which the total strain energy in the molecular and equivalent-continuum models, under identical loading conditions, is equal. The effective mechanical properties of the equivalent-continuum are then determined directly by equating strain energies of the systems. The RVE of a typical nano-structured material is on the nanometer length scale, therefore, the material of the RVE is not continuous, but is an assemblage of many atoms. Interaction of these atoms is described with a molecular-mechanics force field. The molecular model represents the RVE of the equilibrium molecular structure of the nano-structured material.

The geometries of the homogeneous, equivalent-continuum RVE's were assumed to be cylindrical, similar to that of the molecular models. The mechanical properties of the solid-cylinder continuum models were determined by equating the total strain energies of an equivalent-truss and an equivalent-continuum model under identical loading conditions. Once the mechanical properties of the equivalent-continuum RVE's were determined, the composite material RVE's were assumed to behave in the composite as effective fibers and were used in subsequent micromechanical analyses to predict the influence of effective fiber volume fraction, orientation, and length.

Constitutive models of the effective fiber/polymer composites were obtained from a micromechanical analysis by using the mechanical properties of the nanotube/polymer effective fibers and the bulk polymer matrix material. For the composites considered in this study, the polymer molecules that were near the polymer/nanotube interface were included in the effective fiber, and it was assumed that the polymer matrix surrounding the effective fiber had mechanical properties equal to those of bulk polyethylene. It was also assumed that perfect bonding existed between the nanotube/polymer effective fibers and the surrounding polymer matrix in the micromechanics analysis.

The plate buckling equations used to assess the benefits of the SWNT-reinforced polymeric composites considered in the present study are the simple closed-form equations presented by Nemeth for specially orthotropic plates [8], [9]. These equations are for infinitely long plates with a constant thickness (t), a constant width (b), and with either simply supported or clamped edges. The solutions for infinitely long plates are

particularly useful in preliminary design of structural elements because they represent lower bounds to the corresponding festoon buckling-load-versus-plate-aspect-ratio curves for finite-length plates. Moreover, the equations are based on classical plate theory and are for plates that are subjected to uniform axial compression (N_X), uniform shear (N_S), or pure in-plane bending loads (N_B), as shown in Fig. 1.

Classical plate theory assumes that each layer of material is in a state of plane stress. For the single layer of homogenized material considered for the plates herein, the material constitutive relation is given in terms of the nonzero principal-material-direction stresses by where the stiffness matrix, commonly called the reduced stiffness matrix, [Q] and the four independent elastic constants are E_1, E_2, G_{12}, and ν_{12}. For a single-layer orthotropic plate, the bending stiffness matrix [D] is then given by

$$[D] = \frac{t^3}{12}[Q] \tag{1}$$

As is well known, the buckling behavior of thin plates is represented by a fourth-order partial differential equation, with homogeneous boundary conditions. The critical, or buckling, load is found by solving the associated boundary-eigenvalue problem for the smallest value of the applied load. For the three distinct types of in-plane loads considered herein (compression, shear, and bending), the buckling formulas are given in terms of the nondimensional buckling coefficients given by

$$K_X = \frac{N_X^{cr} b^2}{\pi^2 \sqrt{D_{11} D_{22}}} \tag{2}$$

$$K_S = \frac{N_S^{cr} b^2}{\pi^2 \sqrt[4]{D_{11} D_{22}^3}} \tag{3}$$

$$K_B = \frac{N_B^{cr} b^2}{\pi^2 \sqrt{D_{11} D_{22}}} \tag{4}$$

where the superscript *cr* denotes the critical value of the applied load that corresponds to buckling. To make direct comparisons of plate buckling resistance, the buckling coefficients defined herein are not the best choice. It is more useful and convenient to use a buckling load that is nondimensionalized with respect to the bending stiffness of an isotropic plate made of the bulk polymer material.

Results and Concluding Remarks

Computational Materials research at the NASA Langley Research Center proposes to significantly reduce development costs of new nanostructured materials for aerospace applications by bringing physical and microstructural information into the realm of the

design engineer. The intent of the program is to assist the material developer by providing a rational approach to material development and concurrently assist the structural designer by providing an integrated analysis tool that incorporates fundamental material behavior.

The macroscopic buckling resistance of composite plates made of a polyethylene matrix material that is reinforced with single-walled carbon nanotubes has been presented. In particular, the relative influence of molecular structure, nanotube length, and nanotube volume fraction on buckling resistance of infinitely long plates subjected to uniform axial compression, uniform shear, or pure in-plane bending have been quantified for both functionalized and nonfunctionalized nanotubes. A multi-scale analysis method was developed that established constitutive equations by using a hierarchical equivalent-continuum modeling technique that predicted elastic bulk behavior, using intrinsic properties developed through molecular dynamics simulations. The elastic properties of the equivalent continuum were then used in a micromechanics analysis to predict elastic properties of a single-layer specially orthotropic plate as a function of nanotube alignment. The predictions of buckling resistance were based on these resultant elastic properties.

The results presented in figure 2, shows that for a fixed nanotube volume fraction of 1% and various nanotube lengths, the buckling resistance of the random, nonfunctionalized nanotube composite exceeded all other cases with the increase in nondimensional buckling load ranging up to 25% (at nanotube length of 400 nm) when compared to the composites reinforced with the aligned, functionalized nanotubes.

The results that have been presented figure 3 also show that for a fixed nanotube length of 400 nm and various nanotube volume fractions, the buckling resistance of the random nanotube composites exceeded all other cases with the increase in buckling resistance ranging up to 500% (at 40% volume fraction) when compared to the aligned composite. At the large volume fractions, the influence of functionalization was to slightly decrease critical buckling loads.

Based on all the cases considered in the present study, it appears that the use of randomly oriented, nonfunctionalized nanotubes would be recommended when the design criteria is focused on providing the largest possible value of in-plane buckling resistance. The primary elastic properties that influence this result are the composite-plate stiffnesses that correspond to twisting and anticlastic curvature. To achieve the largest gains in buckling resistance, nanotube volume fractions greater than 20% are warranted.

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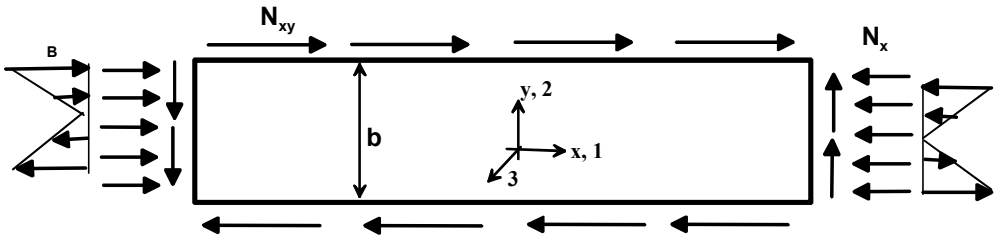

Figure 1. Schematic illustration of the mechanical loads and coordinate directions for the infinitely long, orthotropic plate.

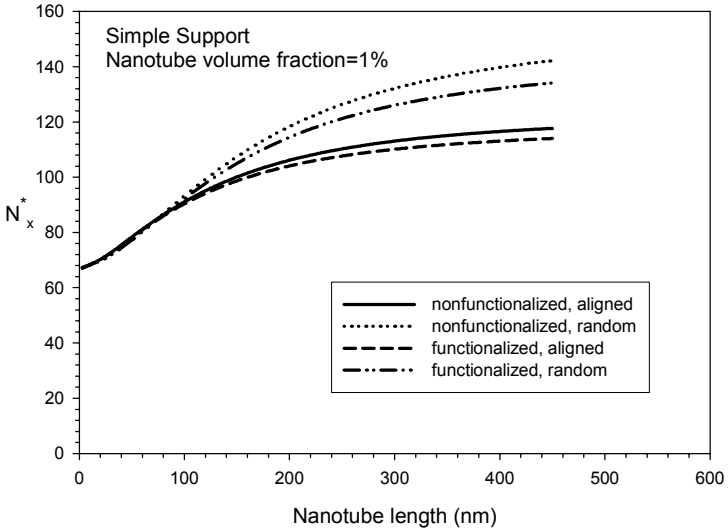

Figure 2: Normalized buckling load for compression, simple support, fixed volume fraction.

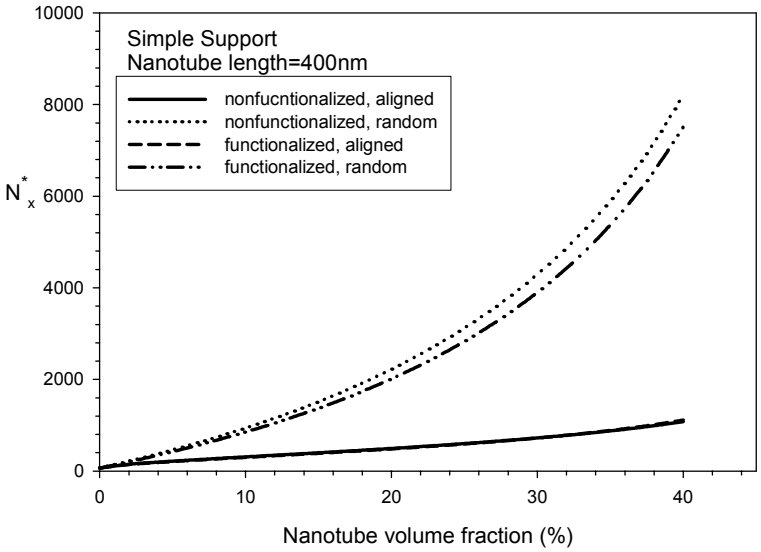

Figure 2: Normalized buckling load for compression, simple support, fixed nanotube length.