Multiscale Modeling and Simulation of Nanoparticle-reinforced Damping Materials

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ABSTRACT

Carbon nanotubes are used in many applications, particularly for vibration damping and noise reducing materials. In the present paper, multiscale computational approaches to modeling of nanoparticle-reinforced composite materials and virtual reality engineering tools have been used to describe/model an intuitive interface of some CNT-reinforced materials to enable efficient design and synthesis of next generation materials and nanoscale devices. The scope is to understand the damping mechanisms in a viscoelastic polymeric medium. In this paper the equilibrium equation of damping structure is described with advanced FEM-based models and is solved with the help of a numerical code created by CASE tools.

Keywords: nanomaterials, dynamics, computations, CASE

1 INTRODUCTION

Nanoparticle/tube/fiber-reinforced composite materials are novel vibration damping solutions entailing placement of numerous nanoscale particles inside a vibrating material structure [1-3]. Carbon nanotubes can be treated as a simple nanoscale spring [1] with some advanced energy dissipation mechanisms, and thus giving a possibility to multiply by billions a damping performance of the next generation engineering materials. However, the mechanisms involved in such materials need to be understood [4, 5]. Multiscale damping modeling/design tools is not readily available.

Our joint group is exploring the use of virtual reality systems and IT technologies (e.g., C++, FEM code, CASE tools such as Rational Rose) for interactive modeling and visualization of nanoparticle-based systems/materials. A computational scheme and software, which utilizes C++ and CASE tools, was developed to predict properties of nanoparticle-reinforced materials, to optimize and control their performance capabilities. An objective of the paper is to demonstrate an application of modern software engineering tools for modeling virtual reality and molecular dynamics of novel nanocomposites.

2 MODELING OF NANOCOMPOSITE

2.1 Aspects of damping mechanics

The CNT-reinforced material damping phenomenon is complex because of friction between nanotube and a matrix and the variety of other energy dissipation/fracture mechanisms involved, and because of the structure of the nanoparticles and material matrix used [5-8], etc. that are affecting a damping. During vibration, nanoparticles interact with material matrix and one another and, thus, dissipate energy through momentum transfer and friction. Some attempts have been successfully made to apply the most commonly used engineering finite element-based approach (FEM) for modelling down to nanoscale [9-13]. However, advanced numerical modelling approach for damping prediction of CNT-reinforced solids was developed [30].

At bending test of CNT/polymer composites [14], nanotubes might be pulled out. Fracture mechanism of multiwalled carbon nanotubes at tensile loading may has telescopic-like transformation mechanism [15-17]. MWNT can be treated as a hard particle (E_{avg}=1GPa) in a softer matrix, acting as a sword-in-sheath where the outer nanotube fractures followed by pullout of the interior walls [15]. In a nanotube composite, where load is transferred through shear stresses at the nanotube/matrix interface, the relatively weak van der Waals bonding between the layers of the nanotube results in almost the entire load being carried by the outer nanotube wall [10-12, 18, 19]. However, both theoretical and experimental investigations have shown the remarkable reversible deformations (up to 40% of their size) of carbon nanotubes in compression, tension and bending [20-22]. Some researchers [11-12] noted that a MWCNT transformation mechanism is between Euler-type buckling for small diameter nanotubes (about 10 nm) and local kinking for larger diameter (above 60 nm) nanotubes. As now on it is not clear that this remarkable resilience at the nanoscale is pertinent in engineering damping applications of composite material at both large and small displacements/stresses and requires further investigations.

2.2 Computer-based algorithm

The modeled object (damping CNT/composite material) can be effectively drawn in diagrams by CASE tools such as "Rational Rose" where key elements are presented as structural units and then are used for generation of programming code [29]. Overall, the Use case (fig. 1) and the Class Diagram (fig. 3) and is the most important for further synthesis of software code. When utilizing an object-oriented design process, it is a common practice to draw a

sequence diagram for each use case. In doing so, objects and messages that are sent between objects are defined by user's options inside of materials and actors outside.

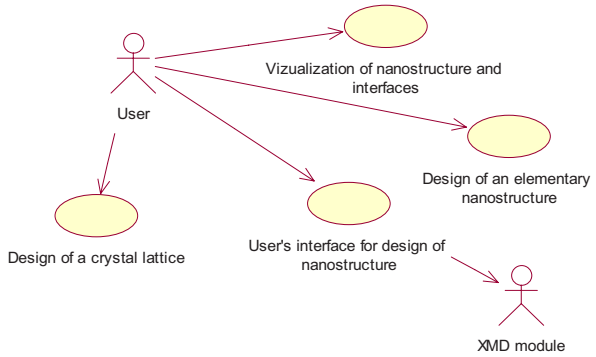

Figure 1: "Use case" diagram for nanoscale modeling.

This is useful for process-intensive applications, for the application described in this paper; this stage was skipped going directly to the class diagram. Class diagram-to-use case conformance was checked throughout the design process to verify that the classes were sufficient to implement the use cases. Designed to be modular and extensible, the engineering workbench for damping can be described by two important concepts, functionality and generality. The architecture functionally divides itself into Model, Input, Output and Manager. Thus other diagrams can be developed. Component diagram is shown in fig. 2, where is databases/modules, is relations between modules.

The module for design of an elementary nanostructure is based on user's data to be chosen from chemical element database or inputted by hands based on type of lattice and basis. The module for design of crystal lattice of damping material interprets the data obtained from the above module and then designs some structure of material matrix. The module for visualization treats the data of the former module and graphically represents structure of the material. There is also the module to provide data transfer from external software. XMD module, which is used for molecular dynamics simulations [28], computed positions of atoms after CNT reinforcement. Then MatLab 7.x and ANSYS 9.x [27], which is based on FEM code, were used for large scale simulation of CNT-reinforced materials, repeating iterations so as to grab necessary engineering data into complex workbench tools.

Based on the Class diagram in Rational Rose environment a user can develop computer code of the class on selected programming language. In MS Visual C++ a user can assess entire hierarchy of MFC library classes by using visualized tools that is called - Model Assistant. At some final stages of workbench development, his modules are implemented in Microsoft Visual C++.

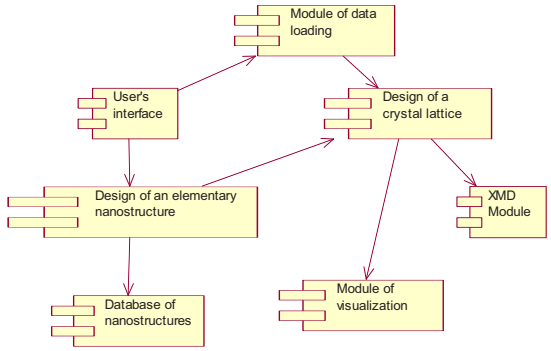

Figure 2: "Component" diagram.

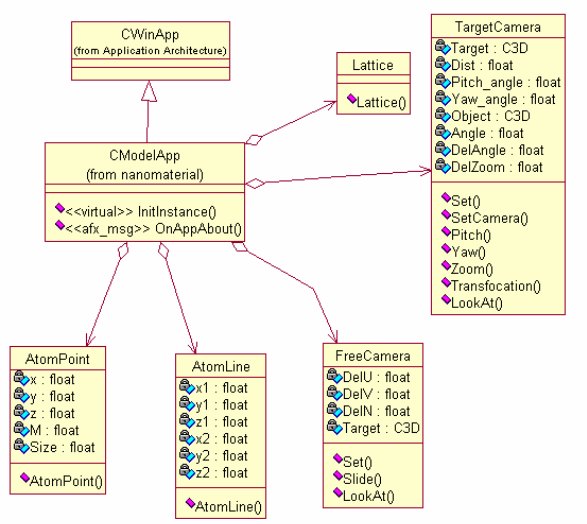

Figure 3: Class diagram for code synthesis.

The positions of all atoms in the atomic lattices can be further calculated and stored in a data file at two regimes: simulation and calculation. Regime of simulation is used for visual design purposes in order to find some optimal orientation, distribution and location of particles in a matrix. The design concept is then being used for computational analysis and calculations of damping/dynamic properties of materials based on affiliated prediction models integrated into database. Virtual database of visual structures and computational tools will introduce outstanding possibilities to researchers in this field.

3 COMPUTATIONAL APPROACH

The dynamic characteristics of the CNT-reinforced structure can be described by its eigenvalues and eigenvectors [23]. These establish the relation between loss factor, damping ratio and the structural deformation. The equilibrium of the damping structure can be described by the fol-

lowing equation in matrix form and then solved by FEM-based approach [9-13] for the 2 degree of freedom system:

$$\begin{bmatrix} m_1 & 0 \\ 0 & m_2 \end{bmatrix} \cdot \Delta \ddot{D}^{n+1} + C^n \cdot \Delta \dot{D}^{n+1} + \left(\begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix} + k_v \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} + ik_v \eta_v \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \cdot \Delta D^{n+1} \right) = \Delta F^{n+1} \quad (1)$$

where superscript n and n+1 are incremental steps; Cn is damping matrix at nth step; vectors ΔDn+1 and ΔFn+1 are displacement and force at (n+1)th step. Average value of surface strain is used to represent structural deformation as shown in [29]. Dissipated energy due to friction is equivalent to the frictional shear force the differential displacement between carbon fibre and a matrix [24].

The full energy dissipation, energy dissipation and loss factor for one loading cycle can be found respectively as follows:

$$U_{diss} = \int_V (\sigma_{ij} \varepsilon_{ij} / 2) dV; \qquad \eta = \arcsin\left(\frac{\Delta U}{2\pi U_{diss}} \right) \quad (2)$$

$$\Delta U = 2\tau^{\max} (2\pi r_n l_n^2) \cdot (\varepsilon_z^m - \varepsilon_z^{\max});$$

where indexes are related to m is matrix material, max is maximum displacement, n is nanoparticle, diss is dissipation energy, ε is strain, and τ is shear stress. Substituting the matrices in the Eq. (1) by corresponding matrices given by the Eqs. (3), the fully integrated set of equations can be obtained for prediction of damping behaviour of the CNT-reinforced system.

The stiffness matrix for the Eq. (1) has been established as shown in [9-13, 26]. The mass and damping matrices of the CNT-reinforced material (Fig. 1e) can be found with the following consideration. If the mass per unit length (m) is constant along the length of material, it can be taken out of the integral equation. The mass matrix of the material is fully populated. If loaded along the axes, Z and assumed two degree of freedom ∫ψbψbdx=L [26], the matrices can be written in the symmetric form as follows:

$$M_2 = m_2 \begin{bmatrix} \int_{a_1}^{a_2} \psi_1 \psi_1 dx & \int_{a_1}^{a_2} \frac{1}{2} \psi_1 \psi_2 dx & \int_{a_1}^{a_2} \frac{(t_2 - 2t_1)}{4} \psi_1 \varphi' dx \\ - & \int_{a_1}^{a_2} \psi_2 \psi_2 dx & \int_{a_1}^{a_2} \frac{(2t_2 - t_1)}{3} \psi_b \psi_b dx \\ - & - & \int_0^L (\varphi\varphi + \frac{(t_1^2 - t_1 t_2 + t_2^2)}{4} \varphi' \varphi') dx \end{bmatrix};$$

$$C = \begin{bmatrix} a_1 E_x (1+\eta_{xi}) & a_1 E_x (1+\eta_{xi}) & a_1 E_x (1+\eta_{xi}) \\ a_1 E_y (1+\eta_{yi}) & a_1 E_y (1+\eta_{yi}) & a_1 E_y (1+\eta_{yi}) \\ a_1 E_z (1+\eta_{zi}) & a_1 E_z (1+\eta_{zi}) & a_1 E_z (1+\eta_{zi}) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad (3)$$

where ν is Poisson ratio in three-dimensional space (x, y, z), a is coefficient defined as follows:

$$a_1 = \frac{1-\nu_1\nu_2}{1-\nu_3^2-2\nu_1\nu_2-2\nu_1\nu_2\nu_3}; \qquad a_2 = \frac{\nu_3+\nu_1\nu_2}{1-\nu_3^2-2\nu_1\nu_2-2\nu_1\nu_2\nu_3};$$

$$a_3 = \frac{1-\nu_3}{1-\nu_3-2\nu_1\nu_2}; \quad a_4 = \frac{1-\nu_1}{1-\nu_3^2-2\nu_1\nu_2}; \quad a_5 = \frac{1-\nu_2}{1-\nu_3^2-2\nu_1\nu_2}$$

4 RESULTS

Resulting picture (fig. 4) of nano simulation shows respectively, for example, crystallise lattice of aluminium matrix, carbon nanoparticles of chosen shape (pyramid, sphere or fullerene-like) and nanocomposites represented as aluminium matrix with two introduced pyramid-like carbon nanoparticles (green-atoms in fig. 4). The positions of all atoms in the atomic lattices are also calculated and stored in a file. The data are used for further calculations of mechanical properties by FEM-based techniques. Virtual database of various nanostructures and their computer-based calculations will introduce outstanding possibilities to researchers in this field. The user can easily attach his hand to an atom or molecule and manoeuvre it in 3D space.

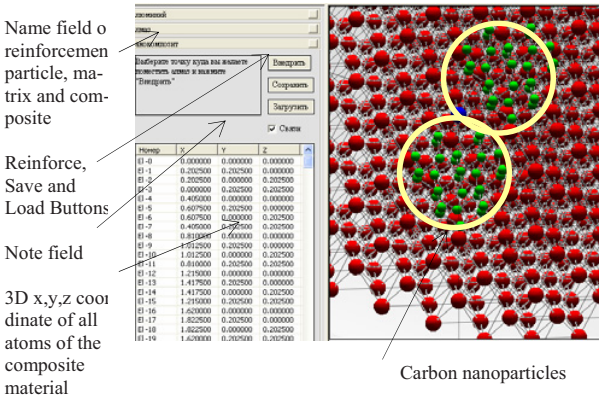

Figure 4: CNT-reinforced nanocomposite.

Damping behavior of CNT-reinforced polymeric material produced according to the technique [26] has been investigated at resonance frequencies between 10Hz and 10,000Hz band. The damping performance was determined by Modal Strain Energy analysis [25] and laser vibrometry, and was compared to the numbers predicted from the Egs. (1-3). Good correlation between the simulations (fig. 5) and some previous researches [26] can further be used as an engineering benchmark tools and a case of support.

It was validated that a concept of using CNT as vibration damping oscillators where CNT acts like a nano-shock-absorber and damping effect can be multiplied by a factor of thousand billions when dispersed in a material matrix. The principal conclusions are that by invoking the properties of nano-auxetics/nanostructures it is possible to control the wave/sound/vibration propagation in the material and

enhance the energy dissipation that can assist in improving the inherent damping of materials, but an experimental/theoretical environment is required to apply it in industry. In this respect developed computational tools and engineering workbench is important part of next generation aerospace design. Results of the project potentially create fundamental basis for investigation and development of 3-D reinforced composite structures with high nanoscale structures volume content, using nano-scale reinforcement architecture to reduce component mass and dimension, enhance performance, and reduce costs.

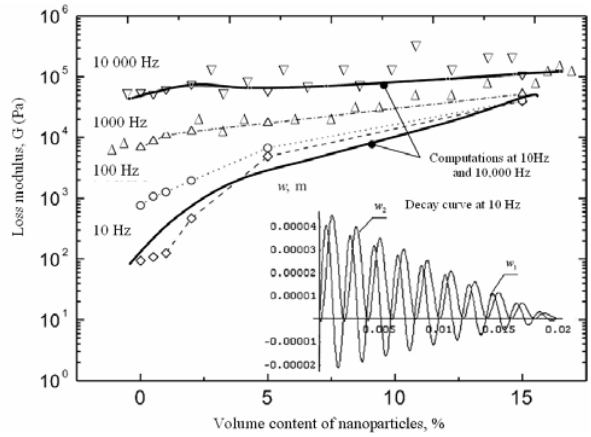

Figure 5: Damping behavior of CNT-reinforced material.

5 CONCLUTION

Computational simulation and modeling tools called also as a Virtual Reality Environment (VRE) can help to understand many damping effects and predict the behavior of damping materials via computer-generated media[1].

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