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Multiscale Modeling of Nano Tube Based Composites and Devices

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Introduction

Due to their unique structural, mechanical, thermal, and electrical properties [1], carbon nanotubes (CNTs) have been proposed as ideal fibers for manufacturing the next generation of composite materials [2] with mechanical and thermal management applications. In addition, it has been demonstrated that CNT-based devices exhibit some interesting and unique characteristics, including a high oscillation frequency [3].

As a powerful tool for elucidating complex physical phenomena, molecular dynamics (MD) was employed to study nanocomposites and nanodevices [4,5]. Since MD cannot simulate large models of nanocomposites and nanodevices, some researchers employed continuum models, including micromechanics models and electromechanical models. However, both MD and continuum approximation have significant limitations with respect to length and time scales. Such limitations prevent one from using those methods in studying numerous phenomena, including material failure and function failure in nanotube-based composites and device systems. Therefore, the development of efficient numerical methods, including multiscale methods [6], capable of addressing various length and time scales is very important for the design and analysis of nanocomposites and nanodevices.

Bridging domain coupling method

As one type of multiscale methods, concurrent multiscale methods employ an appropriate model in different subdomains to treat each length scale simultaneously. The bridging domain coupling method [7] was initially developed to couple different domains with various length scales, mainly the molecular domain and the continuum domain. Figure 1 demonstrates the schematic of the bridging domain coupling method, in which a scaling parameter α is introduced in the bridging domain, i.e. the overlapping subdomain, Ω_0^{int}, between the molecular domain Ω_0^M and the continuum domain Ω_0^C.

Consequently, the total Hamiltonian for the complete domain is taken to be a linear combination of the molecular and continuum Hamiltonians

$$H = (1-\alpha)H^M + \alpha H^C \quad (1)$$

The molecular and continuum models are constrained on the overlapping domain by requiring the atomic displacements to conform to the continuum displacements at the positions of the atoms in the bridging domain. The constraints are applied to all components of the displacements. With the Lagrange multiplier method, the equations of motion can be derived.

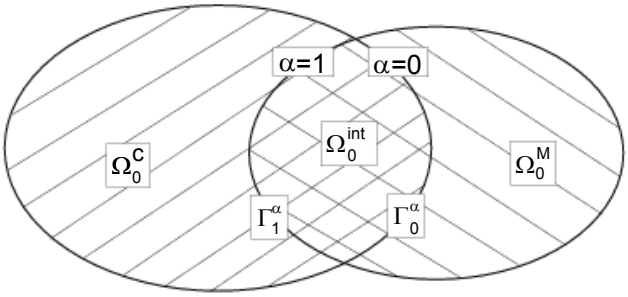

Figure 1: The schematic of the bridging domain coupling method.

An explicit algorithm [7] including a coupling technique in the bridging domain was developed for solving the equations of motion. At first, so-called trial velocities are obtained independently in the continuum and molecular domains without the consideration of constraints. Then, constraints are applied to calculate the Lagrange multipliers. Finally, the constraints are considered to correct the nodal/atom velocities in the bridging domain. This coupling method can eliminate wave reflection automatically [7], and it has been proven to be stable [8]. The bridging domain coupling method can be extended to the bridging domain multiscale method which couples multiple length scales and time scales with the implementation of high performance computing [9].

Nanoscale continuum approximation

Another kind of multiscale methods is called hierarchical multiscale methods. One of the typical hierarchical multiscale methods is the Quasicontinuum (QC) method [10], in which the intrinsic properties of the material are determined at the atomic level and embedded in a continuum model using a homogenization procedure. In this method, the constitutive equation is constructed via the Cauchy-

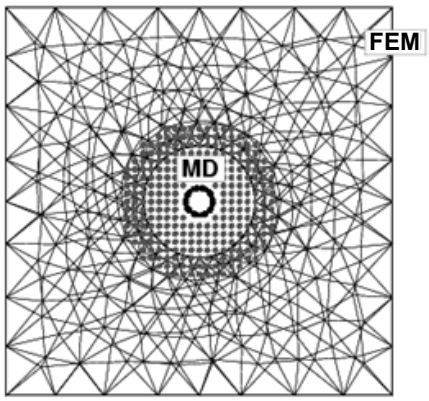

Figure 2: Bridging Domain Coupling Model of SWNT/AL Nano composites (Top View).

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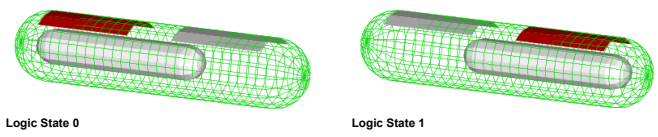

Figure 3: Positions of the inner tube at different logic states in memory configuration.

Born (CB) rule by the QC approach. The CB rule assumes that there are locally homogeneous deformations in the continuum model. Therefore, the atomic-level lattice follows the deformation given by the macroscopically imposed deformation gradient.

Most homogenization techniques including the CB rule provide a link between molecular and continuum models. However, the continuum model is usually assumed to be at a zero temperature. As a result, temperature effects at the nanoscale cannot be investigated via most currently-existed continuum approximation. A temperature-related Cauchy-Born (TCB) rule was developed [11] to enhance multiscale/multiphysics modeling and simulations. In the TCB rule, the Helmholtz free energy, i.e. the effective energy, rather than the potential energy at the nanoscale is considered. The assumptions include: 1) atoms have locally homogeneous deformation; 2) atoms have the same local vibration modes; 3) the vibration of an atom is harmonic; and 4) coupled vibration of different atoms is negligible.

Consequently, the continuum-level first Piola-Kirchhoff stress for continuum approach to finite-temperature nano systems as follows,

$$\mathbf{P}(\mathbf{F},T)=\frac{\partial w_H(\mathbf{F},T)}{\partial \mathbf{F}} \tag{2}$$

where w_H is the free energy density, and it is a function of the deformation gradient and the temperature. Equation (2) can serve as a temperature-dependent constitutive relation that can be implemented in most multiscale methods to investigate temperature-related physical behavior of nanostructured materials and devices.

CNT-embedded composites

CNT-embedded aluminum composites were studied via the bridging domain coupling method [12]. Single-Walled Nanotubes (SWNTs) were considered and assumed that long SWNTs are aligned unidirectionally and distributed homogeneously in the Al matrix. A multiscale unit cell model of nanocomposites is shown in Figure 2. In this multiscale model, the SWNT is embedded in the center of the unit cell. The bridging domain is a circular band between the molecular and continuum models of the Al matrix.

The similar models can be developed for nanocomposites with Multi-Walled Nanotubes (MWNTs) and SWNT bundles. Numerical simulations are conducted to study the strength reinforcement when unit cell models with the same size are considered and CNT volume fractions are the same. It is evident that the MWNT results in the most significant reinforcement, followed by the SWNT bundle. The SWNT results in the least significant reinforcement compared to the other two inclusions.

CNT-based memory cells

The double-walled carbon nantoube-based co-axial oscillators [13] can be extended to design a new NEMS system as memory cells. The outer tube is positioned on the top of a conducting ground plane. Atomic materials for two conducting electrodes are deposited on the top of the outer nanotube. The inner tube sits in a double-bottom electromagnetic potential well. The depth of the potential well under the electrode is proportional to the WRITE voltage applied to the electrode. The induced quasi-static electromagnetic forces exerted on the inner tube will overcome interlayer friction if the applied voltage is sufficiently large. Consequently, lateral motion of the inner tube will be induced as a result. The capacitance of the device gate can be read when a READ voltage is applied. As a result, the logic state of the NEMS gate can be determined. It should be noted that all READ voltages are sufficiently small so that the motion of the inner tube will not be influenced. Whether the inner tube is underneath one electrode or the other will result in two different physical states determined by the READ voltage. These two different physical states can be interpreted as Boolean logic states. Therefore, the system can be used as a random access memory (RAM) cell.

Figure 3 is the nanoscale continuum model of a CNT-based memory cell with two Boolean logic states. Numerical simulations showed that the frequency of the designed RAM can be as high as 6.75 GHz.

Conclusions

Molecular Dynamics has difficulties in modeling and simulating large nano systems. The example of modeling CNT-based nanocomposites shows that the bridging domain coupling method can efficiently simulate large nano systems and investigate physical phenomena at the nanoscale. On the other hand, nanoscale continuum approximation can efficiently model large nano devices. This paper can be viewed as a framework to provide alternative solutions for modeling nanocomposites and nanodevices.

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