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A bridging cell multiscale modeling of carbon nanotube-reinforced aluminum nanocomposites

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ABSTRACT

In this paper, the Young's modulus and failure mechanics of nanotube-reinforced aluminum nanocomposites has been investigated using the Bridging Cell Method (BCM). The advantage of the BCM for multiscale modeling of CNT-Al nanocomposites is in its quasi-static formulations in concurrent multiscale environment with specialized local quasi-harmonic approximations for thermal contributions. The model has been initially verified by coupling the atomistic-continuum domains in a representative volume element of the nanocomposite. The multiscale method sets the nanotubes as part of the atomistic domain, while the rest of the domain is kept in the continuum domain and modeled using the finite element method. The types of nanotube reinforcements considered in this study are single-walled nanotubes (SWNTs), multi-walled nanotubes (MWNTs) and a bundle of SWNTs. It was found that the overall strength of the nanocomposite was similar between the different reinforcements, but the toughening mechanisms differed significantly between the three. The model has been tested for two different crystalline planes in the aluminum crystal to observe the degree of toughening on different atomic planes where it was found that the essential plane and the cleavage plane had similar ultimate tensile strength, however the role of toughening was less prevalent in the cleavage plane case.

1. Introduction

Carbon nanotubes (CNTs) are known to exhibit superior electrical, thermal, chemical and mechanical properties for a wide range of engineering applications [1,2]. The discovery of CNTs in 1991 marked a new age of research due to their enhanced aspect ratios, along with their large tensile strength and thermal conductivity [3,4]. Furthermore, the Young's modulus for such structures has been reported to reach up to 1 TPa. Due to these advanced properties, an attractive use of this material is to fabricate advanced nanocomposites using CNTs as a mechanical, thermal and electrical reinforcement for the utilized material matrix [5,6].

The three main material classes present in CNT composites today are polymers, ceramics and metals. The introduction of CNTs into these matrix materials has enhanced all three classes of composites significantly during the past decade [5]. CNT-polymer composites have utilized the high aspect ratio of nanotubes to enhance their properties through unique interactions of polymer chains crosslinking with CNTs [7]. As a result of this crosslinking, the CNT-matrix interface has been observed to have higher packing, better orientation and enhanced mechanical response. Alternatively, ceramic composites utilize CNTs as a toughening component as ceramics are already considered to have high mechanical strength, but are brittle in fracture [8,9]. The current challenge of CNT-ceramic composites is optimizing fabrication for better dispersion, density and surface quality. Recent research has also aimed to produce multifunctional metal matrix composites (MMC) due to the thermal, electrical and mechanical properties of CNTs. Accredited to the recent advancement in nanotechnology, MMCs reinforced with CNTs have enticed recent interest in modern engineering uses such as wear and friction resistance [10,11], hydrogen storage [12,13], catalytic roles [14,15], aerospace [16,17] and nuclear reactors [18]. Hence, CNTs have been regarded as an ideal filler for diverse types of multifunctional composites.

CNT-nanocomposites are known to experience unique fracture behavior. A study of such fracture behavior would provide better insight into interfacial interactions, load transfer and breakage mechanisms. In particular, the interfacial load is essential in determining the degree of reinforcement of such fillers. This can be achieved by proper embedding of the CNTs within the selected material matrix. The main components of interactions have been identified as weak/non-bonded and covalent bond interactions for the CNT composite [19–21]. As such, molecular dynamics (MD) is regarded as one of the most powerful tools

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for modeling nanoscale interactions for mechanical and thermal property assessment [22–24]. Using MD, load mechanisms along the CNT-matrix interface have been investigated, with enhanced fracture toughness reported to reach up to 200% [25], however in the study presented in Ref. [25], the domain was limited to 1000 atoms, restricting the extent of fracture behavior investigated.

In recent years, multiscale modeling has emerged to overcome the computational load issues of atomistic simulations by enhancing the spatial and temporal coupling on a multitude of material scales [26–28]. Multiscale modeling is generally categorized as either hierarchical [29,30] or concurrent [31,32]. Hierarchical modeling utilizes lower scale simulations to determine larger scale properties in separate runs. Alternatively, two or more material scales exist in the same simulation in concurrent modeling such that a coupling or a handshake region is developed to bridge the two domains. The concurrent model allows for modeling localized damage phenomena as well as non-uniform deformation and simultaneous evaluation of interaction effects propagating into continuum regions. Unfortunately, most concurrent methods enforce a spurious force weighting scheme in the coupling domain to account for the missing neighbor interactions from the atomistic domain [26]. In order to overcome such effects, methods have been developed that rely on novel energy based weighting. One such method is the Bridging Domain Method (BDM), where a study of CNT reinforced aluminum composites has been investigated and showed adequate results but only in a single crystalline plane of aluminum [33]. More recently, a method has been developed to model the whole simulation domain with conventional finite element method (FEM) solvers and is called the Bridging Cell Method (BCM) [34–39]. The advantage of BCM is its quasi-static formulations, where the steady-state behavior is obtained while excluding the temporal scale entirely.

Some researchers have utilized micromechanics to model CNT composites [40–42]. Such micromechanics are possible by hierarchical or cohesive zone modeling to represent the interface between the matrix and the CNT inside the composite. Rafiee et al. has utilized tessellation techniques in order to model aggregates of CNTs within polymer matrices using Meso-scale multiscale modeling [43]. Furthermore, an FEM formulation was utilized to assign each carbon atom bonding as beam elements and a modal analysis was conducted within the micro-scale FEM environment [44]. The same framework was applied to impact and post-impact analyses and to capture structural properties of carbon nanotube reinforced polymer (CNTRP) materials with multiple size ranges of CNTs [45–48]. These techniques performed well for large scale property calculations, structural dynamics and deformation mechanics, however, they are limited when modeling localized regions of nano-sized fracture mechanics, where the discrete atomic nature of CNTs becomes more dominant such that it cannot be considered as a continuum anymore. When this is the case, a molecular model should be incorporated into the fracture simulations. This can only be accomplished when satisfying the de-Broglie hypothesis [49]. Moreover, basic nano-scale continuum mechanics models may be limited when capturing the rupture of atomic bonding. These methods are also restricted when investigating localized deformation mechanics such as dislocations, crack propagation, wave propagation and slip planes at the atomic scale. Likewise, the breakage and toughening mechanisms were not investigated before in a concurrent multiscale simulation with nano-scale domains using a quasi-static loading condition. This would provide vital information regarding the effect of reinforcements against multiple crystalline planes under static loading. For MMC, the deformation mechanism is quite different from ceramic and polymer-based composites. The matrix material here does not experience brittle fracture as ceramics do, but also does not have large viscoelastic deformation with lower temperature and strength thresholds as found in polymers. In MMCs, the addition of CNT reinforcement was found to reduce the ductile deformation regions as the dimple regions in the fracture surface (typical in ductile fracture from crack nucleation and void coalescence) were reduced significantly by CNT fillers [50,51]. It would provide great insight to observe the breakage mechanism and the constitutive relation for such a class of composites in a multiscale framework.

In this article, the BCM is utilized to model the interfacial interactions between the CNT and aluminum matrix while interpreting its strengthening and toughening response with three types of CNT reinforcements. The advantage of BCM is in its quasi-static formulation that captures the exact atomic/discrete nature of CNTs within the molecular model while enforcing thermal contributions with simplified local quasi-harmonic approximations. The work represents the first RVE and nanocomposite simulation of BCM to capture the toughening mechanics on multiple crystalline planes with a quasi-static, concurrent multiscale framework. The CNT and the surrounding metal matrix interface will be placed inside the atomistic domain to accurately observe the interaction area, while the rest of the domain is coupled under FEM formulations. The metal matrix is chosen to be aluminum with Face Centered Cube (FCC) crystalline packing. The next section will outline the BCM formulation and the associated thermal control. Section 3 will include representative volume element (RVE) simulation to verify the existing model. The fracture and toughening behavior of the system is investigated in Section 4 for three types of CNT fillers, followed by conclusion and future recommendations.

2. Bridging Cell Method formulation

The BCM approach discretizes the material domain using bridging cell coupling as shown in Fig. 1. The continuum domain in this study is modeled with conventional static finite element method (FEM) [52,53]. The bridging domain is formulated by obtaining its total energy as a summation of continuum E_B^C and atomistic E_B^A energy contributions as follows:

$$E_B = E_B^C + E_B^A \tag{1}$$

where $E_B^A = \sum_{i\in\Omega^B}^{n_a} \sum_{j\in\Omega^B\cap\Omega^A} U(r_{ij})$ takes into account the energy contributions from the interatomic potential U as a function of the interatomic distance r_{ij} between atom i and j.

The continuum contribution $E_B^C = \sum_{c=1}^{n_c} w_c \cdot W(\nabla_c) \cdot V_c$, for n_c bridging cells, comes from the local strain energy density W, where each node is weighted by a factor as follows:

$$w_c = 1 - \frac{\sum_i R_{ij} U(r_{ij})}{W(\nabla_c) \cdot V_c} \tag{2}$$

where the ratio in the expression represents the atomistic to continuum energies in the current bridging cell and its corresponding nodes. R_{ij} symbolizes the ratio of distances between atoms i and j in the chosen cell.

The atomistic domain is modeled by the Atomic-scale Finite Element Method (AFEM) [54,55]. According to the AFEM, the atomic stiffness matrix K_A and force vector f_A can be obtained with the

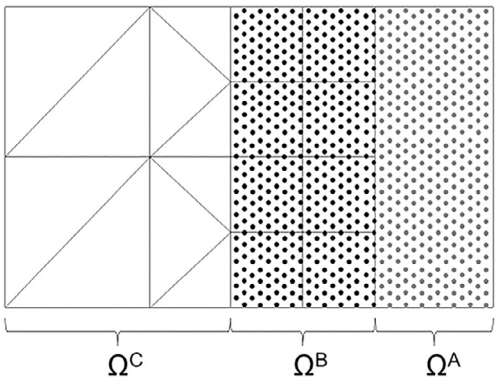

Fig. 1. Domain decomposition of BCM formulation to continuum (Ω^C), bridging (Ω^B) and atomistic (Ω^A) domains.