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CNT-polymer nanocomposites under frictional contact conditions

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ABSTRACT

The unique intrinsic physical properties of Carbon NanoTubes (CNTs) suggest that they are ideal fillers for high-performance composites. Although some experimental studies have revealed the potential of these nanoparticles to tailor the tribological properties of polymer-based composites, the number of theoretical studies on the characterization of their frictional behavior is still very low. This paper is aimed at filling this lacuna by addressing the theoretical analysis of the indentation response of CNT-polymer nanocomposites. To do so, it is first necessary to compute the overall mechanical properties of CNT-polymer composites. Secondly, these properties must be used to evaluate the macroscopic indentation response of the composites. In this work, an extended Mori-Tanaka approach is used to extract the constitutive properties of CNT-polymer nanocomposites. On the basis of ad hoc Eshelby's tensors accounting for particular wavy filler geometries, along with a two-parameter agglomeration model, the homogenization process is performed considering the coupled effect of fillers' waviness and agglomeration. Afterward, a 3D boundary element formulation for contact modeling is applied to study the indentation response of these nanocomposites. The main objective of this paper focuses on analysing the influence of micromechanical features such as fiber content, orientation, waviness, and dispersion on the indentation response of CNT-polymer nanocomposites. Detailed parametric analyses are presented to characterize this phenomenon under frictional contact conditions. The numerical results demonstrate that fillers' waviness and agglomeration have a coupled detrimental effect on the macroscopic response of CNT-reinforced composites.

1. Introduction

In recent years, a broad cross-section of the scientific community has been attracted by Carbon NanoTubes (CNTs) due to their unique intrinsic physical properties. Their remarkable mechanical, thermal and electrical properties open a vast range of applications as reinforcing fillers for high strength composites [1], as well as smart materials with self-sensing capabilities [2–4]. In particular, there exists an increasing interest for the development of polymer-based nanocomposites. Thanks to their excellent corrosion resistance, relatively low unit cost, facile processing and recyclability, polymers are widely used in an extensive and diverse range of tribological areas [5]. The indentation response under frictional contact is a crucial feature for most vital engineering components and systems in industrial applications such as gears, bearings, artificial human joint bearing surfaces, high performance coatings, tires, etc. [6]. The specific development of CNT-polymer nanocomposites allows to obtain new materials with superior indentation resistance and tribological behavior [7,8]. Although some studies have evidenced the promising potential of CNTs to tailor the tribological properties of polymer-based composites, the number of theoretical studies concerning the frictional behavior of carbon nanotube reinforced composites is still very scant.

In this sense, previous studies have shown that Carbon Nanotube-Reinforced Composite (CNTRC) materials exhibit more stable frictional coefficients and lower wear rates [9–12]. Indentation techniques on thin-films and bulk forms have been studied not only to have a better understanding of these materials under contact conditions but also to measure their mechanical properties in CNTRCs [13,14] and in composites doped with Vertically Aligned Carbon Nanotubes (VACNT) [15–20] or with horizontal aligned CNTs [21]. As observed in the tribological response, the indentation response of CNTRCs is highly affected by micromechanical aspects such as alignment and agglomeration. Computational virtual indentation tests allows to characterize the mechanical properties of CNTRCs. In addition, this type of techniques has a great potential to design and maximize the effectiveness of the reinforcement and therefore the properties of the CNTRC. Some works based on the Finite Element Method (FEM) [22–24] have modeled the indentation response of CNTRC. Le and Huang [22] consider explicitly the CNTs and Liu et al. [23,24] assume the effective mechanical properties of nanoreinforced composites. However, as observed in those

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works, a very fine mesh must be considered to approximate CNTs inclusions and the contact problem between the indenter and the specimen. The Boundary Element Method (BEM) [25,26] is recognized as an accurate and efficient numerical tool for studying contact and interface problems. A few works have dealt with the problem of CNTRC modeling using BEM [27–29], taking into account the microstructural approximation of the CNT-polymer system. Although, in all these BEM formulations, no contact indentation conditions were considered.

Recent works on the tribological properties of CNT reinforced polymer composites showed that it would be desirable to control the alignment and the dispersion of the nanoinclusions in the matrix [30,31]. In this context, aligned and well-dispersed CNTs are desirable to develop new advanced composites for more demanding applications and high-performance tribomaterials [21,32,33]. However, due to the electronic configuration of the tube walls of CNTs, as well as their high specific surface area, CNTs tend to agglomerate in bundles resulting in non-homogeneous filler dispersions. In addition, due to their low bending stiffness, CNTs within polymer matrices usually present a certain degree of waviness. Notwithstanding there exists a number of aligning techniques such as the application of magnetic fields [34] and electrospinning [35], as well as dispersing methodologies such as the use of dispersants or sonication, obtaining uniform dispersions of aligned CNTs remains an enormously challenging task. Furthermore, the cost and complexity of these manufacturing processes limit the scalability for this type of configurations [36]. For this reason, the analysis of accurate filler microstructures, including waviness and agglomeration effects, is of pivotal importance for assisting the design of these composites. Despite considerable efforts can be found in the literature on this respect, most studies limit themselves to the study of waviness and agglomeration acting independently.

In light of the previous literature review, this work is aimed at investigating the indentation response of CNTRC under frictional contact conditions with CNT waviness and agglomeration effects. The effective constitutive properties of CNTRCs are predicted by an extended Mori-Tanaka homogenization approach. The agglomeration of CNTs in bundles is analyzed by means of a two-parameter agglomeration model. In addition, an ad hoc Eshelby's approach for accounting for particular wavy filler microstructures. In virtue of the ad hoc definition of the Eshelby's tensor of wavy fillers, it is possible to study the coupled effect of waviness and agglomeration. The analysis of the indentation response of CNTRCs is conducted by a 3D BEM formulation. A contact constitutive friction law for ACNT fibers is considered and incorporated to an augmented Lagrangian contact resolution scheme, which allows us to solve the contact problem taking into account both the mechanical and the tribological anisotropic characteristics (i.e. anisotropic bulk properties and anisotropic wear and frictional conditions). The proposed methodology is applied to study the indentation response of a CNTRC half-space configurations, and how micro and nanomechanics affect the contact compliances. The potential of the present work is illustrated by detailed parametric analyses on the influence of microstructural features such as filler orientations, filler content, as well as the sliding direction and the thickness of the film on the normal and tangential contact forces. Finally, the coupled effect of waviness and agglomeration on the indentation response is investigated. The results demonstrate that both mechanisms have detrimental influence on the overall stiffness and, when act simultaneously, their effect add up. Overall, the present work presents a comprehensive micromechanics-based 3D formulation for the analysis of the tribological response of CNTRCs, including a realistic definition of the microstructural features.

The remainder of this work is organized as follows: Section 2 presents the problem description, Section 3 presents the micromechanical constitutive models for CNTRCs. Section 4 overviews the basic governing equations of the indentation response and the non-linear contact conditions. The literature on BEM formulations is quite extensive, so in Section 5 we briefly present the basic ideas of a boundary element formulation to solve contact problems. Section 6 presents the numerical results and discussion and, finally, Section 7 concludes the paper.

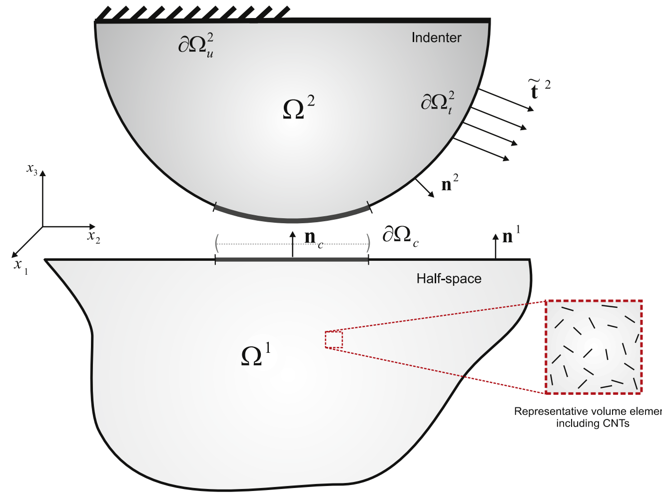

Fig. 1. The physical setting. Domain Ω^1 is the CNT reinforced composite domain and Ω^2 is the indenter.

2. Problem description

Let us consider an elastic half-space Ω^1 and an elastic indentor Ω^2 over in $\mathbb{R}^3$, see Fig. 1. The boundary of Ω^l (l = 1,2), $\partial\Omega^l$, is divided into three disjoint parts: $\partial\Omega_t^l$ with prescribed tractions $\tilde{t}_i^l$ (i = 1,2,3), $\partial\Omega_u^l$ with imposed displacements $\tilde{u}_i^l$ and $\partial\Omega_c^l$ represents the potential contact surfaces, which have outward unit normal vectors n_i^l. Under small displacement and strain assumption, these boundaries are almost coincident (i.e. $\partial\Omega_c^1 \simeq \partial\Omega_c^2$) so we can define a common contact surface $\partial\Omega_c$ with a normal vector $n_{c,i} \simeq n_i^1 \simeq -n_i^2$. Moreover, the infinitesimal strain tensor ε_{ij} can be obtained from derivatives of the displacements field u_i in $\Omega^1 \cup \Omega^2$ as: $\varepsilon_{ij} = (u_{i,j} + u_{j,i})/2$ in $\Omega^1 \cup \Omega^2$.

On the domains Ω^l, assuming static loading conditions, the mechanical equilibrium equations in the absence of body forces are:

$$\begin{aligned} \sigma_{ij,j} &= 0 && \text{in} \quad \Omega^1 \cup \Omega^2, \\ \sigma_{ij} n_j^l &= \tilde{t}_i && \text{on} \quad \partial\Omega_t^1 \cup \partial\Omega_t^2, \\ \sigma_{ij}^1 n_{c,j} = -\sigma_{ij}^2 n_{c,j} &= p_i && \text{on} \quad \partial\Omega_c, \end{aligned} \tag{1}$$

with σ_{ij} being the components of Cauchy stress tensor, n_i the unit normal on $\partial\Omega_t^1 \cup \partial\Omega_t^2$, p_i is the contact traction and σ_{ij}^1 and σ_{ij}^2 are restrictions of σ_{ij} to a particular domain Ω_t^l. In this work, summation convention is adopted unless explicitly stated otherwise (so repeated indexes imply sum). Finally, the stress and strain tensors for a general anisotropic linear elastic material are related through the linear constitutive law as follows:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}, \tag{2}$$

where C_{ijkl} denotes the elastic stiffness tensor, which is positive definite and satisfies the following symmetries: $C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}$.

3. Micromechanics constitutive modeling of CNTRCs

In this work, the macroscopic elastic moduli of CNT-reinfoced polymer composites are computed by mean-field homogenization approaches. In particular, three different filler arrangements are considered, namely composites doped with uniformly distributed straight CNTs in Subsection 3.1, composites doped with uniformly distributed wavy CNTs in Subsection 3.2, and composites doped with heterogeneous dispersions of CNTs in Subsection 3.3. Throughout this section, a boldface letter stands for fourth-order tensor, and a colon between two tensors denotes inner product, $\mathbf{A}:\mathbf{B} \equiv A_{ijkl}B_{klmn}$.

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