



Nonlinear modeling of carbon nanotube composites dissipation due to interfacial stick–slip



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ABSTRACT

A nonlinear constitutive theory is proposed to describe and characterize the hysteretic elastoplastic response of nanocomposite materials caused by the inelastic shear stick–slip between carbon nanotubes and the surrounding matrix. The theory combines the mean-field homogenization method based on the Eshelby equivalent inclusion theory, the Mori–Tanaka homogenization approach, and the concept of inhomogeneous inclusions affected by inelastic eigenstrains. The shear stick–slip is accounted for as an incremental plastic eigenstrain in the inclusions. The evolution of the introduced plastic eigenstrain is regulated by a constitutive law based on a micromechanical adjustment of the von Mises function based on the interfacial stress discontinuity. Parametric studies show that the investigated carbon nanotube composites can exhibit superior damping capacities by determining optimal nano/micro-scale constitutive parameters to maximize the nanofrictional energy dissipation.

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1. Introduction

Nanostructured materials, such as polymeric matrices integrated with carbon nanotubes (CNTs), are used in a variety of applications, ranging from nanocomposites with superior mechanical performance to materials with electromagnetic shielding properties or composites for energy storage (Basiricó and Lanzara, 2012; Formica and Lacarbonara, 2012), to mention but a few. Among the major properties exhibited by nanocomposites, their unique ability to absorb vibrations and noise turns out to be one of the most attractive features in view of various applications in diverse fields of engineering such as aerospace, automotive, and civil engineering. The ability to absorb and dissipate mechanical energy, typically referred to as damping capacity, has become a necessary feature for multifunctional composite structures, such as multi-stable morphing composites, and more general dynamic systems.

In addition to the numerous studies and tests conducted in the last decades on the effective mechanical properties of CNT composite materials (Anumandla and Gibson, 2006; Ashrafi and Hubert, 2006; Chen and Cheng, 2009; Formica et al., 2009; Formica and Lacarbonara, 2009; Gibson, 1994; Kim et al., 2006; Nemat-Nasser and Hori, 1993; Ogasawara et al., 2011; Zhao and Weng, 1990), a considerable amount of experimental data was obtained to either characterize the interfacial CNT–matrix properties or to measure the damping capacity of these promising nanostructured materials (Ajayan et al., 2006; Auad et al., 2009; Ci et al., 2006; Frankland and Harik, 2003; Gibson et al., 2007; Gou et al., 2004; Khan et al., 2011; Rajoria and Jalili, 2004; Suhr et al., 2004; Teo et al., 2007). Indeed, it was proved that a low interfacial shear strength (ISS) between the CNTs and the hosting matrix, in addition to a high interfacial contact area, results in a significant increase of damping capacity (Man et al., 2009; Namilae and Chandra, 2005; Suhr et al., 2005; Sun et al., 2009). Rajoria and Jalili (2005) showed that

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the low adhesion at the nanotubes-polymer interface together with a good alignment and dispersion of the CNTs maximize the damping capacity of the nanocomposites, observing in a series of vibration tests an increase up to 700% of damping ratio in epoxy composites integrated with 5% weight fraction of multi-walled carbon nanotubes. They assumed a stick-slip model to describe the main source of energy dissipation arising from the ability of the CNTs to slide inside the matrix. [Suhr and Koratkar \(2008\)](#) showed how mechanical damping is related to the frictional energy dissipation during interfacial sliding all over the high contact areas between nanotubes and polymeric matrix, and discussed the effects of the applied strain amplitude on the interfacial slippage of CNTs.

Other relevant works extensively investigated the influence of some key parameters on the nanocomposite damping behavior, such as CNT volume fraction, surface treatments for the interfacial adhesion, dispersion and geometry of CNTs, showing that the loss modulus may increase up to 1000% with only 2% weight fraction of SWCNT fillers ([Ajayan et al., 2006; Auad et al., 2009; Li et al., 2009; Slosberg and Kari, 2003](#)).

In the context of the frictional energy dissipation phenomenology, as mentioned, the combination of an extremely large interfacial area – due to the high CNT specific surface area – and the weak bonding between the CNTs – whose length scale is comparable with that of polymeric chains – and the matrix is the key physical aspect that causes high damping ([Kao and Young, 2009](#)), thus emphasizing the importance of constitutive parameters such as the CNT volume fraction and the interfacial shear strength ([Savvas et al., 2012](#)). The phenomenon behind this damping enhancement can be explained by the stick-slip theory as suggested by previous works.

[Zhou et al. \(2004\)](#) developed a stick-slip damping model for aligned, well-dispersed SWCNT/polymer composites extending the stick-slip phenomenon observed at the atomic scale by [Buldum and Lu \(1999\)](#) and [Holscher et al. \(1998\)](#) to the nanotube-resin interface. The damping model was later expanded by [Liu et al. \(2010\)](#) in a three-phase micromechanical model, composed of resin, resin sheath acting as shear transfer zone, and CNT ropes. More recently, an effective model incorporating the stick-slip for unidirectional nanocomposites has been proposed by [Dwaikat et al. \(2011\)](#) to determine the hysteretic energy dissipation. They considered the effects of the CNT volume fraction, aspect ratio and fiber-to-matrix stiffness ratio on the damping capacity, then adopting an optimal set of parameters to maximize the frictional energy dissipation. This result suggested the possibility to design and optimize CNT nanocomposites for advanced damping applications.

Following the same idea of designing ultra-damping materials to meet the high demands for innovative vibration and noise control systems, other interesting friction models for the interfacial energy dissipation in CNT composites have been proposed by [Huang and Tangpong \(2010\)](#) and [Lin and Lu \(2010\)](#).

At the same time, due to their low density, high stiffness and tensile strength, CNTs turn out to be a truly attractive reinforcing agent for metals, polymers or ceramics. This interest inspired the development of constitutive models capable of describing not only the CNT-matrix interface features, but also the overall nonlinear behavior of these nanostructured materials. These models exploited molecular dynamics using both atomistic and continuum theories. Over the past decade, several multi-scale models have been proposed to elucidate the influence of the CNT volume fraction, agglomeration, orientation and interfacial conditions on the overall mechanical properties of CNT composites ([Anumandla and Gibson, 2006; Ashrafi and Hubert, 2006; Frankland and Harik, 2003; Odegard et al., 2003](#)) leading to effective nonlinear elastoplastic constitutive models addressing issues such as agglomeration and load transfer at the CNT-matrix interface ([Ju and Sun, 2001; Sun and Ju, 2001; Sun et al., 2013; Weng, 2009; Yang et al., 2013](#)).

Among these works, the relevant study of [Barai and Weng \(2011\)](#) deals with the elastoplasticity of CNT composites described by a two-scale model, where an imperfect interface (spring-like) model is adopted at the smaller scale. Moreover, starting from the early works of [Hill \(1965\)](#) and [Mori and Tanaka \(1973\)](#), incremental elastoplastic meso-mechanical constitutive models were later developed. In particular, [Gonzalez and Llorca \(2000\)](#) adopted the self-consistent method to compute the elastoplastic behavior of a two-phase material considering the effects of a stress redistribution due to damage evolution, while [Doghri and Ouair \(2003\)](#) proposed a new incremental homogenization formulation featuring consistent tangent and secant operators to analyze the cyclic deformation of composite materials. These rich analytical models have been recently extended in the works of [Doghri et al. \(2010\)](#), [Guo et al. \(2013\)](#), [Pierard et al. \(2007\)](#) by developing finer cyclic viscoplastic constitutive models to describe hysteretic behaviors.

Finally, interesting attempts have been pursued to develop models that may incorporate dissipative mechanical features of the nanocomposites, including the multi-scale, mass-spring model ([Fraternali et al., 2011](#)) for foam materials integrated by carpets of unidirectional CNTs, where the dynamic dissipation shown by the material under cyclic compressive loading is accompanied by hysteresis and strain localization. The macroscopic hysteresis is interpreted as a rate-independent phenomenon that describes the damping and elastoplastic behavior of the nanocomposite.

The present paper proposes a step forward from these initial works, in the attempt to provide effective predictive tools by which the damping due to interfacial frictional sliding between CNTs and matrix can be accurately described. In particular, a theoretical framework is proposed for the elastodynamic response of CNT nanocomposites, accounting for their eminently nonlinear material behavior. Furthermore, the resulting model is intentionally constructed to be easily and efficiently implemented in standard finite element computational codes.

In particular, the presented meso-scale nonlinear incremental constitutive theory is a combination of the mean-field homogenization method based on the Eshelby equivalent inclusion method ([Eshelby, 1957, 1959](#)), the Mori-Tanaka homogenization based on the concept of average stress and strain ([Benveniste, 1987; Mori and Tanaka, 1973](#)), and the idea of Mura of inhomogeneous inclusions with inelastic eigenstrains ([Mura, 1987](#)). Hence, we leverage on the idea of introducing inelastic eigenstrains to model the shear stick-slip between CNTs and matrix. The evolution of the plastic eigenstrains is regulated

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