European Journal of Mechanics A/Solids 64 (2017) 112–130

Contents lists available at ScienceDirect

European Journal of Mechanics A/Solids

journal homepage: www.elsevier.com/locate/ejmsol

Computational micromechanics analysis of electron hopping and interfacial damage induced piezoresistive response in carbon nanotube-polymer nanocomposites subjected to cyclic loading conditions

A.K. Chaurasia [a], G.D. Seidel [b, a, *]

[a] Department of Engineering Science and Mechanics, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, USA
[b] Department of Aerospace and Ocean Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, USA

A R T I C L E I N F O

Article history:
Received 5 March 2015
Received in revised form
16 January 2017
Accepted 4 February 2017
Available online 14 February 2017

A B S T R A C T

The current computational multiscale micromechanics based exploration of sensing capabilities in carbon nanotube (CNT)-polymer nanocomposites focuses on the macroscale piezoresistive response when the nanocomposite is subjected to cyclic loading conditions. It has been shown that electron hopping at the nanoscale is the primary mechanism behind the observed macroscale piezoresistivity for such nanocomposites. A continuum description of the non-continuum electron hopping effect used in the current work enables the use of multiscale continuum micromechanics based approaches to study nanocomposite piezoresistivity. The focus of the current work is on the interfacial separation/damage initiation, evolution and accumulation when subjected to cyclic loading. Interfacial separation/damage is allowed at the nanoscale CNT-polymer interface using electromechanical cohesive zones. The mechanical response of the CNT-polymer interface is obtained in terms of normal/tangential traction-separation behavior from atomistic scale Molecular Dynamics based models reported in the literature. The coupled electrostatic response is based on evolving interfacial resistance through the electron hopping induced current density across the separated interface. It is observed that the effective macroscale piezoresistive response obtained from the current modeling framework captures interfacial separation/damage state and shows sensitivity to damage accumulation over several cycles of applied strains.

1. Introduction

Carbon nanotubes (CNTs) have been identified and explored over the past two decades as exceptional nanofillers for nanocomposites with improved mechanical, electrical and thermal properties. More recently, the multifunctional response of CNT-polymer nanocomposites has captured the imagination of the scientific community. The multifunctionality refers to coupled response, e.g. electromechanical or thermomechanical, which has opened up a range of applications for such nanocomposites in several emerging areas (Gibson, 2010). In particular, CNT-polymer nanocomposites have been observed to exhibit an effective piezoresistive response i.e. changes in electrical resistance when subjected to deformation (Boger et al., 2008; Gao et al., 2009; Kang et al., 2006a, 2006b; Loh et al., 2005; Song et al., 2009; Veedu et al., 2006; Watkins et al., 2004; Zhang et al., 2006). The observed piezoresistivity in CNT-polymer nanocomposites has led to experimental and computational investigation of CNT-polymer nanocomposites for structural health monitoring applications (Boger et al., 2008; Dang et al., 2008; de la Vega et al., 2012; Fernberg et al., 2009; Gao et al., 2009; Heeder et al., 2012; Kang et al., 2006b, 2009; Ku-Herrera and Aviles, 2012; Li and Chou, 2008; Loh et al., 2005; Lu et al., 2007; Oliva-Aviles et al., 2011; Park et al., 2008; Song et al., 2009; Thostenson and Chou, 2006; Wichmann et al., 2009; Zhang et al., 2006). Recent advances in techniques for tailoring the microstructure of CNT-polymer nanocomposites have presented the possibility of fabricating structural members with inherent strain/damage sensing capability owing to the observed piezoresistive response (Boger et al.,

* Corresponding author. Kevin T. Crofton Department of Aerospace and Ocean Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061, USA.
E-mail address: gary.seidel@vt.edu (G.D. Seidel).

http://dx.doi.org/10.1016/j.euromechsol.2017.02.002
0997-7538/

2008; Veedu et al., 2006). However, the observed macroscale piezoresistivity is attributed to mechanisms originating at the nanoscale and transitioning though complex interactions at the microscale into the observed macroscale response. Thus, in order to develop systems capable of identifying the of strain/damage state based on the macroscale piezoresistive response, a detailed understanding of the various factors affecting macroscale piezoresistivity need to be examined starting at the nanoscale where complex interactions between individual CNTs and CNT-polymer interfaces lead to effective macroscale response.

The macroscale effective change in resistance of the CNT-polymer nanocomposites in response to applied strains is believed to be attributed primarily to four factors: 1) to the formation and disruption of conductive pathways (Li and Chou, 2008; Theodosiou and Saravanos, 2010) due to the changing nanotube network in the matrix medium. 2) to electron hopping (or quantum tunneling) which is the ability of electrons residing on a nanotube to jump to an adjacent nanotube even when they are not directly in contact (Du et al., 2004; Hua et al., 2008; Li and Chou, 2008; Li et al., 2007; Sun and Song, 2009; Yin et al., 2011; Yu et al., 2010) 3) to inherent CNT piezoresistivity i.e. changes in CNT resistance on application of axial or bending deformation (Cao et al., 2003; Megalini et al., 2009; Rochefort et al., 1999; Theodosiou and Saravanos, 2009, 2010; Tombler et al., 2000) 4) damage initiation and evolution at the underlying scales (Boger et al., 2008; Fernberg et al., 2009; Gao et al., 2009; Ku-Herrera et al., 2013; Li and Chou, 2008; Thostenson and Chou, 2006). Out of these factors, inherent CNT piezoresistivity has been shown to have a small influence on the macroscale effective piezoresistive response in some recent studies (Ren and Seidel, 2012a, 2012b, 2012c, 2013a).

Computational modeling of piezoresistivity in CNT-polymer nanocomposites in the literature is primarily focused at exploring the effect of microscale random CNT/CNT bundle networks and the associated piezoresistivity (Hu et al., 2012; Kuronuma et al., 2012; Li and Chou, 2008; Li et al., 2007; Theodosiou and Saravanos, 2010). Most of these models idealize the CNTs as deformable or rigid stick members dispersed randomly in a polymer medium. These models convert the randomly distributed CNTs into a resistor network accounting for intertube electron hopping using resistors of varying resistance based on the intertube distances. Typically, the electron hopping between the nanotubes is modeled using Simmon's relation (Simmons, 1963) to assess the intertube resistance between CNTs separated by a polymer layer. The evolution of randomly dispersed CNT/CNT bundle network and the associated resistor network leads to observed changes in effective resistance. Some other computational studies (Chaurasia and Seidel, 2014; Chaurasia and Seidel, 2013) have focused on developing micromechanics based models allowing for evolution of electron hopping induced conductive pathways between the CNTs at the nanoscale within the continuum mechanics framework. The conductivity of the intertube region is modified at every incremental strain step to account for evolving electron hopping pathways. The local electric fields and current density in the nanoscale representative volume element (RVE) are solved for using finite element techniques. Finally, electrostatic energy equivalence based micromechanics methods (homogenization) are used to find the effective nanocomposite conductivity as a function of applied strain which is converted to a more appreciable form of piezoresistive gauge factors at the macroscale.

The macroscale effective piezoresistive response is observed to be dependent on the maximum electron hopping range, local volume fraction, macroscale induced local strain state and the magnitude of applied strain. In an attempt to allow for interfacial separation and damage at the nanoscale, the continuum micromechanics based computational model has been extended (Chaurasia et al., 2014) to include the response of the CNT-polymer interface using electromechanical cohesive zones (Blackman et al., 2003; Li et al., 2005; Needleman, 1987; Seidel et al., 2005; Xie and Waas, 2006). The mechanical response of the interface is obtained based on an Molecular Dynamics (MD) based study of CNT-polymer interface RVE conducted by Li and Seidel (Li and Seidel, 2011), which is then inserted hierarchically into the cohesive zone finite element model within the computational micromechanics framework. The coupled electrostatic response of the interface is hypothesized based on arguments about the effective interface resistance associated with polymer ligaments connecting the separated interface. The study, however, only focused on monotonic loading conditions for differentiating the strain and interfacial damage based piezoresistive response.

Several experimental studies have attempted to characterize the piezoresistive response of CNT-polymer nanocomposites (Cravanzola et al., 2013; de la Vega et al., 2011; Kang et al., 2009; Ku-Herrera and Aviles, 2012; Nofar et al., 2009; Wichmann et al., 2009; Yin et al., 2011; Zhang et al., 2013) and CNT doped fiber reinforced composite laminates (Gao et al., 2009, 2010) under cyclic loading conditions. Ku-Herrera and Aviles (2012) applied small number of quasi-static cyclic tensile loading within small deformation range on multi-walled CNT (MWCNT)-vinyl ester nanocomposite samples and observed close correlation between the applied strains and change in macroscale resistance. It was further observed that there is insignificant lag or hysteresis in the piezoresistive response for the small applied tensile strains. Nofar et al. (2009). applied a larger number of strain cycles on MWCNT-epoxy nanocomposites and observed that the residual change in nanocomposite resistance in the undeformed state increases with the number of strain cycles, indicating that the nanocomposite damage can be correlated to the change in macroscale resistance for CNT-polymer nanocomposites. In both of these studies, the maximum strain amplitude was constant. Vega et al. (de la Vega et al., 2011). applied cyclic strains on single-walled CNT(SWCNT)-epoxy nanocomposites with incrementally increasing maximum strain amplitude. They observed that the relative change in resistance increases with increasing strain amplitude in addition to hysteresis effect i.e. the difference in loading/unloading paths. The authors attributed the observed response to interfacial separation at the CNT-polymer interface.

In the current work, the focus is on studying the effect of cyclic loading conditions and exploring the role of interfacial damage initiation, evolution and accumulation in the macroscale effective piezoresistive response for the nanocomposites within the computational micromechanics framework. The nanoscale CNT-polymer interface is modeled using electromechanical cohesive zones to allow for surface tractions and current density across the separated interface developed in (Chaurasia et al., 2014). It is expected that the loading and unloading paths of the cohesive zones at the interface within the non-homogeneous microstructure will lead to damage accumulation at the nanoscale CNT-polymer interface when subjected to cyclic loading. The current work aims to capture these complex interactions at the interface, damage accumulation and the subsequent evolution of the effective piezoresistive response.

2. Model description

Carbon nanotube (CNT)-polymer nanocomposite architecture contains features which span a range of length scales. At the macroscale, the nanocomposite may be considered to be a homogeneous material medium with local properties representative of homogenized subscale microstructural features. At the microscale, the structural features of the nanocomposite start to appear in the