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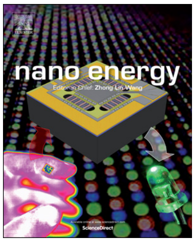

RAPID COMMUNICATION

A multiscale approach to nanocomposite electrical generators

Kasra Momeni

Engineering Mechanics, Iowa State University, Ames, IA 50011, USA

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Abstract

A multiscale approach is pursued to develop a modified shear-lag model for capturing size-scale effects on electrostatic potential generated by a zinc oxide (ZnO) nanowire (NW) in a nanocomposite electrical generator (NCEG). The size-scale effect on elastic modulus of ZnO NWs is captured using a core-surface model. Closed form of governing equations is derived considering linear elasticity for axisymmetric problem and cylindrical coordinate system. Two different configurations based on parallel and series connecting of NCEGs for application in NEMS/MEMS devices are also studied. Parametric studies are performed for sample cases to demonstrate application of the developed model. It is shown that aspect ratio and diameter of NWs are crucial controlling parameters for determining the performance of nanocomposite electrical generators. Numerical results disclose that there is an optimum aspect ratio for each NW of specific diameter. It was also shown that despite the symmetry of loading with respect to mid-plane normal to the NW's axis, the electric potential is not symmetric.

Introduction

The emerging field of nanopiezotronics [1] has attracted the attention of research community to ZnO and in particular its one-dimensional (1D) nanostructures. Zinc oxide NWs have superior mechanical properties relative to bulk ZnO [2,3], large aspect ratio, and low production cost. These properties give ZnO NWs advantages over its bulk form, for energy harvesting applications. Different designs are proposed for nanogenerators to harvest ambient energy using ZnO NWs. The primary configuration of nanogenerators consisted of bended ZnO NWs [4], and multiscale devices based on arrays of these nanostructures were fabricated later [5]. Analytical models [6] and finite element modeling technique have also been utilized to demonstrate the generation of electric potential in ZnO NWs [7]. Although scaling effects in individual ZnO nanostructures were captured using continuum [8] as well as atomistic simulations [9], understanding the scaling effects in complex hierarchical NEMS/MEMS devices is still a challenge. In this paper a multiscale model is developed to address the latter problem and determine the scaling effects on performance of hierarchical nanogenerators.

Size-scale effect on piezoelectric response of nanostructures has been the subject of many research studies. Experimental investigations revealed direct relation between the dielectric constant of ZnO NWs and their lateral size [10]. Continuum models were used for capturing the surface effects on dynamic behavior of piezoelectric nanofilms [11], vibration

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E-mail address: kmomeni@iastate.edu

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and electromechanical response of piezoelectric 1D nanostructures [12]. Simulations including *ab initio* methods and molecular dynamics technique have been utilized to study the size effect on piezoelectric property of 1D ZnO nanostructures [13,14,9]. Significant enhancement in electromechanical response of thin ZnO NWs with diameters smaller than 1 nm was reported [9], due to surface reconfiguration of these nano-sized structures.

A number of energy harvesting devices have been fabricated by connecting arrays of ZnO NWs to take advantage of their unique enhanced piezoelectric properties [15,16]. The design of these devices can be classified into two categories, (i) transversally loaded nanogenerators and (ii) axially loaded ones. Although transversally loaded nanogenerators were fabricated first, latter nanogenerators including NCEGs are based on the axially loaded design. It has been demonstrated that axially loaded configuration has advantages over the transversally loaded ones, including higher electric potential stability, sustainability, and durability [15]. Despite the reports on the modeling [15] and fabrication [16] of NCEG, effect of size scale on their performance has not been well understood.

The load transfer between polymer matrix and ZnO NWs is another factor that plays a key role in determining the performance of NCEGs. Experimental [17] and theoretical [18,19] studies have been performed on the load transfer mechanism between matrix and reinforcement phase, including traditional [20] as well as nanoscale [21] reinforcement phases.

In this study, the shear-lag model proposed by Cox [20] and later developed by Gao et al [21] is modified to capture the size-scale effect on electromechanical response of NCEGs. It is illustrated that aspect ratio and diameter of NWs are the characteristic parameters and determine the performance of NCEGs. Numerical simulations suggest enhancement of electromechanical response by increasing the diameter of NWs, as well as presence of an optimum aspect ratio for each NW of fixed diameter. Although the loading is symmetric with respect to the mid-plane normal to the axis of NW, distribution of generated electric potential is not symmetric with respect to this plane.

The reminder of this paper is organized as follows: First, core-surface model for NWs under tensile loading is elaborated. Second, the piezoelectric behavior of ZnO NWs were modeled using continuum mechanics and linear piezoelectricity. Then, a representative volume element (RVE) was considered for modeling the overall electromechanical response of the NCEG under tension. Governing partial differential equation of generated electrostatic potential was solved numerically for a number of ZnO NWs with different aspect-ratios and diameters. Finally, the numerical simulations analyzed and conclusions on key characteristics of NWs are summarized.

Model development

The ZnO NWs and epoxy matrix are the basic constituent elements of the NCEGs, which are considered to be elastic and perfectly bonded. Although ZnO NWs are orthotropic materials with hexagonal cross-section, here they are modeled as cylindrical structures with isotropic mechanical properties to make the equations analytically tractable. The piezoelectric properties are still modeled with full materials orthotropic symmetry. It was shown that this assumption has only a minor effect on the final conclusions [6].

To model the NCEGs, a cylindrical RVE is considered as shown in Figure 1. Size-scale effects are captured through a core-surface model for elastic modulus of NWs while surface piezoelectricity is neglected [6,15]. The ZnO NWs were modeled as linear piezoelectric materials, and a perturbation technique is utilized to decouple their electrical and mechanical response. The general unitless governing differential equation of generated electric potential in NCEGs is derived in cylindrical coordinate system. It is shown that the governing partial differential equation does not have an explicit analytical solution and numerical techniques must be utilized to solve this equation.

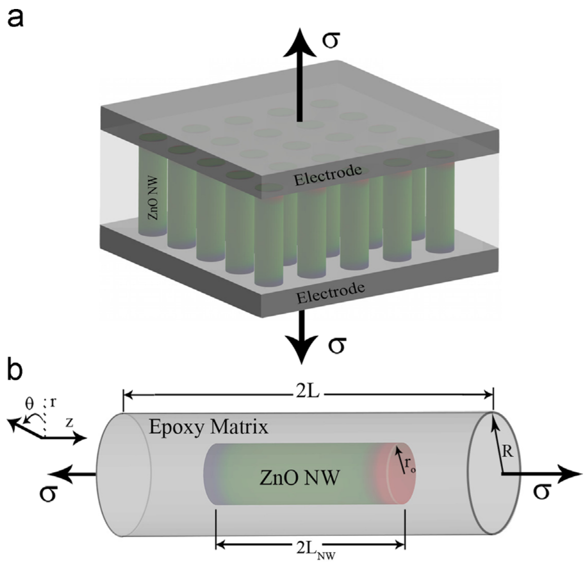

Figure 1 Schematic of NCEG and its corresponding RVE. (a) Schematic of the basic elements of NCEGs, which constitutes an array of ZnO NWs embedded in an epoxy matrix with attached electrodes. (b) The corresponding RVE used for deriving the governing equations of generated electric potential. It constitutes a ZnO NW with length $2L_{NW}$ and radius r_o with axis along the axis of cylindrical surrounding epoxy matrix of length $2L$ and radius R under an axial stress, σ.

Core-surface model

Scaling and surface effects on elastic properties of materials are well studied using continuum mechanics approach [22]. Surface (interface) stresses were modeled as the work (energy) per unit area necessary for stretching the surface (interface) [23]. The core-surface model uses a scaling factor to capture the size-dependent properties of nanomaterials and deviation of their properties from bulk. In this approach NWs are considered as composite structure of a core with bulk properties, designated by subscript *c*, surrounded by a zero-thickness surface, designated by subscript *sr*, with size-dependent properties [24].

The surface effects in epoxy matrix and at the interface with ZnO NWs have been neglected. Such surface effects are strong functions of matrix material and its bonding nature. This may also affect the matrix/NW bonding