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Modeling the material structure and couple stress effects of nanocrystalline silicon beams for pull-in and bio-mass sensing applications

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ABSTRACT

Designed devices for pull-in and bio-mass sensing applications are usually composed of elastic micro/nano-sized beams made of nanostructured materials, such as nanocrystalline silicon (Nc-Si). In addition to the higher-order deformations that ever present in these beams, their material properties are highly affected with the heterogeneity features of their material structure. Neglecting one of these inherent parameters in the modeling of these systems can result in inaccurate predictions of their behaviors. In this research study, the effects of the material structure along with the microstructure couple stress of an electrostatically-actuated micro/nanocantilever beam, made of Nc-Si, on its pull-instability and sensitivity to bio-cells are investigated. Considering the material structure inhomogeneity of the Nc-Si and the beam's size, we propose a novel model that combines a couple stress based-Euler–Bernoulli beam theory and a micromechanical model. To account for the beam's size effect, the modified couple stress theory is used. The heterogeneity nature of the material structure is modeled using a size-dependent micromechanical model that includes the interface and the grain size effects. Performing a parametric study, the results show that including the effects of the material structure and couple stress strongly affects the pull-in voltage values and the estimated masses of the bio-cells. Unlike the couple stress effects, it is demonstrated that the inhomogeneity nature of the material structure softens the beam and hence decreases its natural frequency and pull-in voltage. It is also shown that the couple stress effect enhances the sensitivity of the bio-mass sensor unlike the interface and the grain size effects. The results show that using higher-order modes leads to a significant enhancement in the sensitivity of the bio-mass sensor.

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1. Introduction

Micro/nano structures have received significant interests due to their potentials as sensitive and high frequency devices for applications in Micro-Electro-Mechanical Systems (MEMS) and Nano-Electro-Mechanical Systems (NEMS). Recently, for biological, chemical, and physical applications, micro/nanostructures-based sensors are widely used due to their high sensitivity that can be effectively used in mass detection of biological cells or molecules. Usually, these sensors are composed of an attractor attached to a mechanical resonator whose resonant frequency or deflection is shifted due to the attracted small mass. Due to their large dynamic range, micro/nano-cantilever beams have shown great impacts in biomass sensing applications [1–4]. Moreover, due to their reduced sizes, it is allowed to achieve femtogram ($1fg = 10^{-15}$ g) [1,5], attogram ($1ag = 10^{-18}$ g) [6], and zeptogram ($1zg = 10^{-21}$ g) [7] resolutions.

Recent experimental studies have investigated the effectiveness of micro/nano-cantilevers in mass sensing applications. Burg et al. [8] and Park et al. [9] proposed two novel microfluidic devices to estimate the mass of a single living cell inside a microchannel using micro-cantilevers as bio-mass sensors. Indeed, the mass of the living cell is assessed by detecting the resonant frequency shift of the micro-cantilever. Grigore et al. [10] proposed micro-cantilever-paddles with magnetic resonating elements suitable for application in molecular probe chemistry. Monchev et al. [11] used cantilever sensors to measure the concentration of volatile analytes (water, ethanol, acetone, and ammonia vapors) in air.

The sensitivity of the cantilever mass sensors could be enhanced by using higher order frequency modes and by reducing the size of the cantilever as reported by Narducci et al. [12]. Moreover, controlling the damping rate and the frequency ratio for excited cantilevers can enhance the sensitivity of the mechanical

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resonator [13]. Electrostatically- or piezoelectrically-actuated cantilever beams have shown enhanced sensitivity of the resonant frequency shift to variations in the added mass [14–17]. In electrostatically-actuated sensors, the applied electric voltage between the two electrodes produces an electrostatic force that excites the micro/nano-cantilever beam with an initial disturbance such that the shift in the resonant frequency of the beam could be simply measured with high efficiency. Electrostatically-actuated micro-cantilevers have shown the ability to measure very small frequency shifts when compared to ambient-derived micro-cantilevers [18]. Furthermore, due to their high quality factor values, the resonant frequency of electrostatically-actuated cantilevers could be easily detected which enhances the accuracy of the bio-mass sensor.

Controlling experiments at the nanoscale is difficult and needs qualified labs with expensive costs, the issue which is not available everywhere. At the mean time, various atomistic-based techniques, such as molecular dynamics have shown good contributions to model the dynamic behaviors of MEMS and NEMS devices [19,20]. The molecular dynamics, however, is limited to systems with small number of atoms and is time consuming [21]. On the other hand, modeling MEMS and NEMS devices at the continuum level is distinguished by its low computational cost when compared with molecular dynamics and it is much cheaper than performing experimental investigations.

The existing research studies in the literature that focused on dynamic analysis of micro/nanoresonators are based on using the classical elasticity theories of continua. For example, the classical Euler–Bernoulli beam model is used to investigate the linear and nonlinear dynamics of mass sensors made of micro-cantilever beams [17,18,22]. In the context of the classical elasticity, the cantilever beam is modeled as a continuum consisting of an infinite number of small material particles (represented as mass points) assuming a homogeneous structure of the beam material. However, as a consequence of the decreased size of the cantilever beam, the material particle has to be modeled as a volume element containing certain inner structure. Therefore, the classical elasticity theories have to be adapted for the continuum size effects. Some higher-order elasticity theories have been developed to this purpose by introducing additional material constants to the conventional ones. Several studies have been developed on the mechanical behavior of nano-sized beams, tubes, sheets, and plates using one of these non-classical higher-order theories [23–26]. In Cosserat theories, as higher-order elasticity theories, three additional degrees of freedom for the continuum microstructure rigid rotation are incorporated [27]. In strain gradient theories [28,29], the strain and its gradients contribute to the continuum deformation energy. The modified couple stress theory [30], is a Cosserat-type continuum theory in which an additional material parameter is introduced to capture the microstructure rigid rotation effect on the continuum deformation. The modified couple stress theory is used to investigate the size-dependent responses of the forced vibrational micro-beams [31] and the pull-in instability of electrically actuated micro/nano-beams [32–34] and the results reveal the significant effect of the microstructure rigid rotation on the beam behavior and performance.

On the material structure level, another issue which has to be considered in studying the dynamic behaviors of mass sensors is the heterogeneity nature of the material structure [35–37]. Usually, mass sensors require micro/nano-sized resonators, such as beams and plates. These micro/nano-resonators, as a consequence, are made from nano-structured materials including nano-particle composites, nano-porous materials, and nanocrystalline materials [35–37]. The most dominant characteristics of nano-structured materials are the ultra-small inhomogeneity sizes and the ultra-high specific interface areas (interfaces between the different components of the material structure) [38]. For more illustration, most of polycrystalline materials have heterogeneous inner structures composed of different phases with different volume fractions; grain phase, pores (voids), free-atom cloud phase, etc. In conventional materials (with coarse grains), the most dominant phase with the highest volume fraction is the grain phase. Therefore, in the context of continuum mechanics, representing the structure of conventional materials as a one-phase structure (homogenous) is valid. On the other hand, for example, nanocrystalline materials (NcMs) are polycrystalline materials with grain (crystal) sizes ranging from 1 to 100 nm. Due to the extremely small dimensions of grains, a large volume fraction (e.g. up to 40%) of atoms reside in the interface regions forming an atom-cloud phase. Due to misfits and interactions between adjacent crystallites of random orientations, the atomic structure in the interface regions is distinctly different from the perfect lattice in the interiors of grains [39]. Thus, representing NcMs as homogenous materials is not convenient. Consequently, the heterogeneity nature of the material structure should be modeled by representing it as a composite consisting of a crystal (inclusion) phase with regular lattice connected by an amorphous-like matrix phase (the interface between grains). In addition, due to the intensive decrease in the size of grains of NcMs, the surface to volume ratio of the grain increases, consequently the surface energy has a significant contribution to their overall mechanical properties [38]. In the interior of grains, atoms are bonded from all directions with neighboring atoms unlike those at the free surface of the grain which are only under coordinated forming a coherent grain boundary. Therefore, the average atomic distances between atoms at the grain free surface differ from those between atoms in the interior of the grain. Hence, atoms at the free surface form another distinct phase with different material parameters.

Some investigations have been proposed to illustrate the inhomogeneity size effects on the elasto-plastic properties of nanostructured materials. Kim and Bush [40] and Zhou et al. [41] proposed a phase mixture model in which NcMs are treated as a mixture of crystalline phase, intercrystalline phases (grain boundary, triple line junction and quadratic node), and pores in order to investigate the effects of grain size and porosity on their elastic moduli. Wang et al. [42] studied the impact of the distinct interface on the elastic moduli of NcMs by representing it as a two-phase composite composed of a grain phase and an interface phase. Duan et al. [43] proposed a micromechanical procedure taking into account the surface energy effects on the effective elastic moduli of heterogeneous solids containing nano-inhomogeneities. Zhang et al. [38] proposed a nonlinear micromechanics model to explore the surface effects on the elasto-plastic properties of nano-porous materials and nano-composites. These investigations reflect a decrease in elastic modulus of NcMs with a decrease in the grain size.

In our previous research studies [35–37], a size-dependent micromechanical model have been proposed to model the material structure of micro/nanosolids made of NcMs. This model is harnessed to study the effects of the grain size on the static-bending behavior of beams [35] and the static pull-in instability behavior of electrostatically actuated beams made of nanocrystalline silicon [36]. In addition, a mechanical resonator with a tip mass have been modeled and used for estimating the material structure properties of nanocrystalline silicon and nanocrystalline diamond and used for disease diagnosis [37]. In this research study, we propose a novel model in which the material structure along with the microstructure couple stress is considered. Our objective is to investigate the effects of the material structure inhomogeneity of the Nc-Si and the size of an electrostatically-actuated micro/nano-cantilever beam with a tip mass on its pull-instability, natural frequencies, and sensitivity to measure the