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Investigation of the vibrational behavior and stability characteristics of single-walled zinc sulfide nanotubes

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ABSTRACT

The molecular mechanics is combined here with density functional theory to develop an accurate model for single-walled zinc sulfide nanotubes. It is shown that based on the resemblance between nanotubes and space frame structures, nanotubes can be modeled as a combination of beam and mass elements. Using the developed model, the vibrational behavior and stability characteristics of single-walled zinc sulfide nanotubes with different geometries and under different boundary conditions are investigated. It is observed that the side length of nanotubes affect its vibrational behavior. However, this effect will reduce for longer nanotubes. Besides, it is shown that the stability of nanotubes have a strong dependence on geometry parameters for short nanotubes. However, for sufficiently long nanotube this dependence would diminish.

1. Introduction

Having a wide band gape, 3.8 eV at (300 K) [1], zinc sulfide is considered as one of the most favorable semiconductor materials with the potential applications in nonlinear optical devices, displays, sensors, infrared windows, and lasers [2–4]. Hence, considerable efforts have been done to synthesize ZnS nanostructures such as nanoparticles, nanorods, nanowires and nanosheets [5–9]. Lan et al. [6]

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fabricated ZnS nanorods of diameters 40 to 80*nm* and lengths up to several micrometers by annealing precursor ZnS nanoparticles. Based on thermal evaporation of ZnS powders onto a silicon substrate with the presence of Au catalyst, Wang et al. [8] synthesized single-crystal ZnS nanowires. They used vapor–liquid–solid (VLS) mechanism to control the growth of ZnS nanowires.

Due to exceptional properties of hollow structures, such as nanotubes, including toughness [10], flexibility [11], electronic properties [12], ionic conductivity [13] and anti-hydroxyl radical effects [14], several works have been done to fabricate ZnS nanotubes [15–20]. To utilize these materials, the mechanical properties of them are required to be known. As the properties of materials at the nanoscale differ from bulk properties, these properties should be obtained for nanomaterials. Since the experiments at nanoscale are extremely difficult to be controlled, the theoretical methods have been used extensively. These methods can be classified as atomistic [21–24] and continuum mechanics approaches [25–39].

Relative to carbon nanostructures, there are limited theoretical works have been done investigation of the mechanical behavior of ZnS nanostructures. Using nanoindentation, Yang et al. [40] investigated the nanomechanical deformation of ZnS nanobelts. They found that that the contact stiffness is proportional to the indentation load. However, the elastic deformation of the ZnS nanobelts is independent of sizes. Observing indentation-induced fracture in the nanoindentation of the ZnS nanobelts, they suggested an approach to control nanobelts for the fabrication of nanodevices. Employing direct nanoindentation experiments at room temperature, Li et al. [41] investigated the mechanical properties of ZnS nanobelts. They reported that the hardness of ZnS nanobelts is 79% higher than that of bulk, however the elastic modulus of nanobelts is 52% less than that of bulk material. They observed that nanobelts experiences creep under indentation with the cracks form along the belt growth direction.

Two of the most important methods which have been used to model the atomic interactions of materials are quantum mechanics and molecular mechanics approaches. Quantum mechanics uses the calculations of electronic structure of molecules to propose a model which despite of its accuracy and exerting the simplifications is computationally expensive and time-consuming. In molecular mechanics, ignoring the movements of electrons, a function of nuclear positions is used to describe the system energy. Using this function, although decreases the expensiveness of solution, will result in decreasing the accuracy. So the molecular mechanics will be joined to density functional theory to have a more accurate solution.

In this paper, based on the resemblance between nanotubes and space frame structures, a 3D finite element model have been proposed for single-walled zinc sulfide nanotubes (SWZnSNTs) in which bonds and atoms of nanotubes are simulated by beam and mass elements, respectively. The molecular mechanics combined with density functional theory will be used to derive the elastic properties of these beam elements. The proposed model would be employed to investigate the vibration and buckling behavior of SWZnSNTs.

2. Molecular mechanics modeling

In molecular mechanics the sum of bonded or bonded and non-bonded interactions is used to state the total potential energy of system [42–45].

$$E_t = U_\rho + U_\theta + U_\omega + U_\tau + U_{vdw} + U_{es} \tag{1}$$

where the energies of bond stretching, bond angle variation, bond inversion, and torsion are shown as U_ρ, U_θ, U_ω, and U_τ, respectively and U_{vdw} and U_{es} show the energies of van der Waals and electrostatic interactions, respectively. The specific functional form which is used for these energy terms is specified by material and loading conditions. In the present study, it is expected that the considerable part of potential energy comes from U_ρ, U_θ and U_ω and as the single-walled nanotube is considered, the U_{vdw} will be ignored. Utilizing the Hook's law, which its efficiency and precision in explaining the behavior of atoms under small deformation has been proven [44], for describing the interactions between bound atoms in the system, the Eq. (1) can be rewritten as:

$$E_t = \sum \frac{1}{2} K_\rho (\Delta r)^2 + \sum \frac{1}{2} C_\theta (\Delta\theta)^2 + \sum \frac{1}{2} C_\omega (\Delta\emptyset)^2 \tag{2}$$