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VIBRATIONS OF NANOSTRUCTURES

*** Fernando Ramirez[1], Paul R. Heyliger[2], Anthony K. Rappe[3] and Robert Leisure[4]**

[1]Universidad de los Andes
Civil and Env. Engineering Dept.
Bogota, Colombia
framirez@uniandes.edu.co
www.uniandes.edu.co

[2]Colorado State University
Dept. of Civil Engineering
Fort Collins, CO 80523, USA
prh@engr.colostate.edu
www.engr.colostate.edu

[3]Colorado State University
Department of Chemistry
Fort Collins, CO 80523, USA
rappe@lamar.colostate.edu
www.engr.colostate.edu

[4]Colorado State University
Department of Physics
Fort Collins, CO 80523, USA
leisure@lamar.colostate.edu
www.engr.colostate.edu

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ABSTRACT

One of the most important characteristics of nanostructures is the size-dependence that the properties of these materials and components exhibit. Because of the extremely small size of these structures, the development of efficient methods to evaluate their electronic, mechanical, optical, and acoustical properties is a challenge to researchers. Different analytical methods are available for the determination of the properties of nanostructures including atomistic models and elastic continuum model theories. Atomistic approaches include both quantum mechanics and molecular dynamics and mechanics. In principle, these are the most suitable methods to deal with molecular or atomic motions. However, the application of atomistic models is computationally expensive. Conversely, continuum mechanics approaches are computationally much faster, but they do not explicitly consider atomic and electronic interactions that can affect the properties of these novel structures. At very small length scales, the validity of classical continuum approaches must be evaluated and potentially modified. Nanoparticles show optical and acoustic properties different from those of the bulk crystals of the same material. These differences are mainly attributed to the three-dimensional confinement of electrons and holes in small volumes known as quantum size effect[1], and to the fact that most of the atoms are near the particle surface for these small sizes. Optical properties of nanoparticles have attracted much interest due to their application as optical processing devices and semiconductor lasers. Several studies exist in which the acoustic modes of spherical nanoparticles embedded in a matrix are experimentally measured using Raman scattering. In these studies [2−4] frequency results were analyzed and compared to results obtained using continuum elasticity methods, good general agreement was reported.

In the present study[5], the natural vibration frequencies and modes of free standing silicon (Si) nanoparticles, with sizes ranging from 0.732 to 4.223 nm, were calculated using two different methods: molecular mechanics at the atomic level, and classical elasticity at the continuum level. Molecular mechanics (MM) is a simple atomistic model for molecular structures. Atoms are connected by bonds that can be stretched or compressed due to intra- or inter-molecular forces. MM evaluates the potential energy, V, for a molecular system as the sum of energies from two, three, and four-body interactions, and the kinetic energy from the sum of the contributions of the N atoms forming the molecular system. Vibrational frequencies are calculated by first determining the equilibrium geometry from energy minimization and then replacing the expressions for the total potential and kinetic energies into the Euler-Lagrange equation

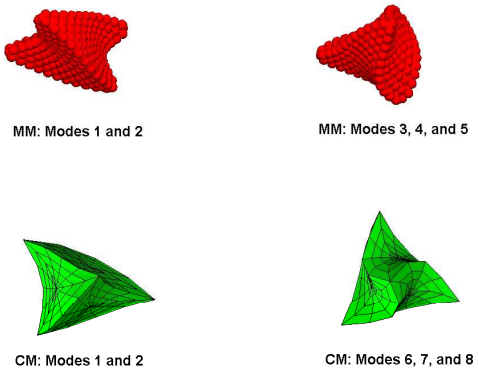

Figure 1: Identical vibrational modes of tetrahedron-shaped nanostructures obtained using molecular mechanics (MM), and continuum mechanics (CM).

which leads to an eigenvalue problem. At the continuum level, the computation of the vibrational spectra begins with the equations of motion for a general anisotropic linearly elastic solid. Following the standard formulation used in variational solid mechanics methods, and assuming harmonic motion for the approximation functions of the displacements also result in an eigenvalue problem to be solved for the natural frequencies and vibrational modes of the corresponding solid. Three different geometries are studied: cubes, spheres, and tetrahedrons. Once the frequency spectra have been obtained, vibrational frequencies and modal shapes obtained from both methods are compared, and the presence and number of degenerate modes are analyzed. Equations describing the variation of the natural frequencies as a function of the particle size and number of atoms forming the nanoparticles are also constructed, for general use. Results indicated that for the range of particle sizes considered (0.732 to 4.223 nm) frequencies are not proportional to the inverse particle diameter as reported in the literature for other nanoparticles, and the frequency-radius product ωR is not scale invariant as it is for continuum elastic solids. The rate at which the nanoparticle frequencies approach the bulk value depends on the particle shape. For all three shapes studied, an estimate is provided of the size of the nanoparticle at which the continuum approach breaks down. Advantage of these facts might be taken in important applications such as the detection of particles smaller than 4 nm, and the evaluation of the mechanical properties of nanostructures. Continuum mechanics methods provide good estimates of the lowest natural frequency of particles having at least 836 (R$>$1.5 nm) and 800 (R$>$1.28 nm) atoms for cube- and tetrahedron-shaped nanostructures, respectively. The vibrational modes obtained from both methods were practically the same for the sphere- and tetrahedron-shaped particles with a large number of atoms (see Fig. 1). In general, vibrational modes shapes obtained using both methods are the same although the order in which they appear may be shifted.

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