ELSEVIER

Engineering Analysis with Boundary Elements 30 (2006) 925–939

ENGINEERING ANALYSIS with BOUNDARY ELEMENTS

www.elsevier.com/locate/enganabound

A Lagrangian approach for quantum-mechanical electrostatic analysis of deformable silicon nanostructures

G. Li, N.R. Aluru*

Department of Mechanical Science and Engineering, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

Received 7 January 2006; accepted 12 March 2006
Available online 18 September 2006

Abstract

Semiconductor mechanical components of nanoelectromechanical systems (NEMS) typically undergo deformations when subjected to electrostatic forces. Computational analysis of electrostatic NEMS requires an electrostatic analysis to compute the electrostatic forces acting on the nanomechanical structures and a mechanical analysis to compute the deformation of the nanomechanical structures. Typically, the mechanical analysis is performed by a Lagrangian approach using the undeformed position of the structures. However, the electrostatic analysis is performed by using the deformed position of the nanostructures. The electrostatic analysis on the deformed position of the nanostructures requires updating the geometry of the structures during each iteration. In this paper, based on a recently proposed hybrid BIE/Poisson/Schrödinger approach, we propose Lagrangian formulations for the BIE/Poisson/Schrödinger equations and solve the coupled Lagrangian BIE/Poisson/Schrödinger's equations self-consistently using the undeformed position of the semiconductors to compute the charge distributions on the deformed semiconductors. The proposed approach eliminates the requirement of updating the geometry and, consequently, significantly simplifies the procedure of coupled electromechanical analysis of NEMS.

Keywords: Lagrangian electrostatics; Quantum-mechanical electrostatic analysis; Nanoelectromechanical systems (NEMS)

1. Introduction

A number of nanoelectromechanical device and system (NEMS) applications have been proposed recently [1–3]. Computational analysis of electrostatically actuated NEMS requires a self-consistent analysis of the coupled electrostatic and mechanical energy domains [4]. Typically, a NEM system contains a deformable and a fixed structure separated by a dielectric medium. The deformable structure is typically made of a semiconductor material, such as silicon, and the fixed structure can be either a conductor or a semiconductor. When a voltage is applied between the deformable and the fixed structures, electrostatic forces act on both the structures due to the induced charges. Since the fixed structure cannot move, the electrostatic forces move only the deformable structure. When the deformable semiconductor structure undergoes a shape change, the charge redistributes in the structure and, consequently, the resultant electrostatic forces and the deformation of the structure also change. This process continues until an equilibrium state is reached. The primary steps involved in the self-consistent solution approach are summarized in Algorithm 1.

Algorithm 1. Procedure for coupled electromechanical analysis

repeat
1. Do mechanical analysis (on the undeformed geometry) to compute structural displacements
2. Update the geometry of the semiconductor using the computed displacements
3. Compute charge distribution in the semiconductor by electrostatic analysis (on the deformed geometry)
4. Compute electrostatic forces (on the deformed geometry)

*Corresponding author.
E-mail address: aluru@uiuc.edu (N.R. Aluru).
URL: http://www.uiuc.edu/~aluru.

0955-7997/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.enganabound.2006.03.012

5. Transform electrostatic forces to the original undeformed configuration
until an equilibrium state is reached

In microelectromechanical systems (MEMS), the mechanical components are typically treated as conductors [5–9] and the electrostatic analysis of MEMS can be performed by solving the potential or the Laplace equation in the domain exterior to all the conductors. However, as the characteristic length in NEM structures can be comparable to the Debye length, the NEM structures can no longer be approximated as conductors. In addition, when the characteristic length of the NEM structure shrinks to several tens of nanometers, the carrier quantum confinement in the semiconductor structure [10] can impose a significant effect on the charge distribution in the mechanical components of NEMS. As a result, coupled Poisson/Schrödinger equations need to be solved self-consistently to obtain the electronic properties such as the potential field and the charge distribution of the system [11,12]. Recently, we have proposed a hybrid BIE/Poisson/Schrödinger approach for quantum-mechanical electrostatic analysis of NEMS [13].

An important aspect of NEMS is that NEM structures typically undergo deformations when subjected to electrostatic forces. The computational analysis of NEMS involves repeated mechanical and electrostatic analysis on NEM structures, as shown in Algorithm 1. The mechanical analysis is typically carried out in the undeformed configuration of the structures. However, the electrostatic analysis is typically performed on the deformed structures. Therefore, the geometry of the structures needs to be updated before an electrostatic analysis is performed during each iteration. The need to update the geometry of the structures could introduce several problems—First, flat surfaces of the structures in the initial configuration can become curved due to deformation. This requires the development of complex integration schemes on curved panels [14] to perform electrostatic analysis. Second, when the structure undergoes a very large deformation, remeshing the surface as well as the interior of the deformed structure may become necessary before an electrostatic analysis is performed. Third, interpolation functions, used in many numerical methods, need to be recomputed whenever the geometry changes. Each of these issues significantly increases the computational effort making the self-consistent analysis of electrostatic NEMS an extremely complex and challenging task. A Lagrangian approach for electrostatic analysis of deformable conductors or MEMS has been proposed and discussed in [6,8,15]. In this paper, we propose a Lagrangian formulation for the hybrid BIE/Poisson/Schrödinger equations for electrostatic analysis of deformable semiconductor nanostructures or NEMS. We refer to this approach as the Lagrangian BIE/Poisson/Schrödinger approach. The Lagrangian BIE/Poisson/Schrödinger approach eliminates the requirement of a cut-off box as well as the requirement of updating the geometry of nanostructures. While the Lagrangian approach is mathematically equivalent to the deformed configuration BIE/Poisson/Schrödinger approach, it significantly simplifies the coupled electrical and mechanical analysis procedure as shown in Algorithm 2. In addition, to take advantage of the flexibility of meshless methods (see e.g., [16]), in this paper we employ the meshless finite cloud method (FCM) [17–20] for interior analysis (i.e., for the solution of the Lagrangian Poisson/Schrödinger equations in the semiconductor) and the meshless boundary integral formulation [21–24] for exterior analysis (i.e., for the solution of the Lagrangian boundary integral equations of the exterior potential equation). The charge distribution and the capacitance of the NEMS are obtained by solving the coupled system of equations self-consistently. Since the primary focus of this paper is Lagrangian electrostatic analysis, based on quantum-mechanical models, we assume that the deformation of the nanostructure is known, i.e., we address the question of if the structure were to undergo a certain deformation, can we compute the charge density without updating the geometry (i.e., we discuss step 2 of Algorithm 2 assuming step 1 can be implemented using existing tools and techniques). For self-consistent mechanical and electrostatic analysis, the deformation can be computed by performing a mechanical analysis using classical theories [7], or classical theories with material properties extracted from atomistic simulation [4], or by using a multiscale approach [25].

Algorithm 2. Procedure for coupled electromechanical analysis by using a Lagrangian approach for both mechanical and electrostatic analysis

repeat
1. Do mechanical analysis (on the undeformed geometry) to compute structural displacements
2. Compute charge distribution in the semiconductor by electrostatic analysis (on the undeformed geometry)
3. Compute electrostatic forces (on the undeformed geometry)
until an equilibrium state is reached

The rest of the paper is organized as follows: Section 2 presents a brief description of the hybrid BIE/Poisson/Schrödinger approach for electrostatic analysis of nanostructures, Section 3 presents the Lagrangian hybrid BIE/Poisson/Schrödinger formulations, Section 4 describes the numerical implementation of the Lagrangian hybrid BIE/Poisson approach, Section 5 presents numerical results and Section 6 presents conclusions.

2. Hybrid BIE/Poisson/Schrödinger approach

To explain electrostatic analysis of NEMS, we consider a nanoswitch example as shown in Fig. 1. The nanoswitch consists of a semiconductor beam structure that is clamped