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Deflection and pull-in instability of nanoscale beams in liquid electrolytes

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ABSTRACT

An elastic beam suspended horizontally over a substrate in liquid electrolyte was subjected to electric, osmotic, and van der Waals forces. The problem, which is governed by four non-dimensional parameters, was solved using the finite element method. The sum of the electric and osmotic forces, the electrochemical force, is usually attractive. However, the electrochemical force can be repulsive for a narrow range of the ion concentration, the initial separation and surface potentials. Furthermore, the beam deflection is not a monotonic function of the applied surface potentials, the bulk ion concentration, or the initial separation between the beam and the substrate. As these parameters are increased monotonically, the beam bends up and then down. The pull-in voltage increases as the bulk ion concentration increases. The pull-in voltage of a double-wall carbon nanotube suspended over a graphite substrate in liquid can be less than or greater than the pull-in voltage in air, depending on the bulk ion concentration. The critical separation between the DWCNT and the substrate increases with the bulk ion concentration. However, for a given bulk ion concentration, the critical separation is independent of the electric potentials. Furthermore, the critical separation is approximately equal in liquid and air.

1. Introduction

Micro and nanofabrication processes are planar technologies. Therefore, many micro and nanodevices consist of beams and plates suspended horizontally over a substrate. On the microscale, suspended beams serve as the active component of accelerometers, rate gyroscopes, pressure sensors, chemical sensors, switches, electrostatic actuators, valves, and pumps. It is reasonable to assume that suspended beams will play a similarly important role on the nanoscale.

van der Waals forces and electrostatic forces are important in the mechanics of nanoscale objects. In gas or vacuum, parallel plate electrostatic actuators undergo a "snap-down" or "pull-in" instability in which the two electrodes spontaneously come into contact when the distance between the two actuators is less than 2/3 of the initial distance. A study of these "pull-in" instabilities is provided in a sequence of papers by Degani and Nemirovsky [1]. Actuators similar to parallel plate actuators have been extended to the nanoscale. Kim and Lieber [2] developed "nanotweezer" NEMS based on carbon nanotubes for manipulation and interrogation of nanostructures. The tweezers have two carbon nanotubes attached to a glass rod. The potential difference between the two carbon nanotubes produces an attractive electrostatic force that can overcome the elastic restoring force of the carbon nanotubes in closing the tweezers. The nanotweezers were used to manipulate polystyrene nanoclusters containing fluorescent dye molecules. Akita and Nakayama [3] performed similar experiments and analysis for nanotweezers consisting of carbon nanotubes in an AFM. Two nanotube arms were fixed on the silicon cantilever tips used as the substrate of the nanotweezers for the AFM. Dequesnes et al. [4] analytically studied the pull-in instability of carbon nanotube switches, which are essentially tweezers, using a continuum model for three coupled energies: the elastic energy, the van der Waals energy, and the electrostatic energy. Rotkin [5] considered the effect of the van der Waals force on the pull-in instability and obtained analytical expressions for the pull-in gap and voltage of a general model. Lin and Zhao [6] studied the dynamic behavior of nanoscale electrostatic actuators by considering the effect of the van der Waals force. A one degree of freedom lumped parameter model was used in these investigations. Ramezani et al. [7] used a distributed parameter model to investigate the pull-in parameters of a cantilever type nanoscale electrostatic switch including the van der Waals force.

In liquid electrolytes, the interaction of electric double layers alters the electrostatic force and also introduces an osmotic force. A number of researchers have modeled the mechanics of two electrodes, separated by nanometers, using discrete springs subjected to electric, osmotic, and van der Waals forces. The primary motivation for this work is the use of atomic force microscopy to measure the forces between solid surfaces in liquid electrolytes, in which the AFM cantilever beam is modeled as a discrete spring. These experiments are usually performed to measure the zeta potential and/or

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determine force–distance or force–voltage relations [8–14]. However, voltage–distance relations are necessary to design electrostatic actuators that operate in liquid electrolytes. Boyd and Kim [15] recently provided voltage–distance relations for nanoscale electrostatic actuators in liquid electrolytes. However, the spring was modeled as a discrete element, not a continuous elastic structure.

The authors believe that the research presented herein is the first study of nanoscale beams in liquid electrolytes in which the beam is modeled as a continuous elastic structure acted upon by electric, osmotic forces, and van der Waals forces. Our objectives are to identify the non-dimensional parameters that govern the beam deflection and pull-in instability, and then determine the critical values of ion concentration and surface potential that will cause the pull-in instability.

The governing equations are presented in Section 2. Results for a gas or vacuum are compared to published solutions in Section 3. For a liquid, novel results are presented in Section 4. Non-dimensional solutions neglecting the van der Waals force are provided in Section 4.1. Solutions including the van der Waals force for a silicon switch and double-wall carbon nanotube switch are presented in Sections 4.2 and 4.3.

2. Governing equations

Fig. 1 depicts a cantilever beam separated from a fixed substrate by a liquid electrolyte. The beam is assumed to be prismatic, homogeneous, and comprised of an isotropic linear elastic material.

The beam is modeled using simple beam theory, also known as Euler–Bernoulli beam theory

$$\tilde{E}I\frac{\mathrm{d}^4u}{\mathrm{d}x^4} = f_{\mathrm{vdW}} + f_{\mathrm{EC}} \tag{1}$$

where u is the deflection of the beam, x is the position along the beam measured from the clamped end, w is the width of the beam, t is the thickness of the beam, I is the moment of inertia about the z axis, and $\tilde{E}$ is the effective modulus. The effective modulus $\tilde{E}$ becomes the Young's modulus E for narrow beams ($w < 5t$) and becomes the plate modulus $E/(1-\nu^2)$, for wide beam ($w \geqslant 5t$), where ν is the Poisson ratio [16]. f_{vdW} and f_{EC} are the van der Waals and electrochemical force per unit length of the beam, respectively. In the present paper, the term "electrochemical force" is defined as the sum of the electric and osmotic forces. The boundary conditions are

$$u(0) = \frac{\mathrm{d}u(0)}{\mathrm{d}x} = 0 \tag{2}$$

$$\frac{\mathrm{d}^2u(L)}{\mathrm{d}x^2} = \frac{\mathrm{d}^3u(L)}{\mathrm{d}x^3} = 0 \tag{3}$$

The van der Waals force per unit length between two parallel plates is given by

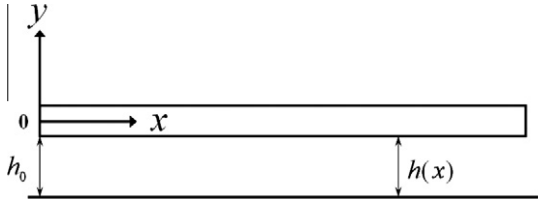

Fig. 1. Nanocantilever beam.

$$f_{\mathrm{vdW}} = -\frac{A_{\mathrm{h}}w}{6\pi(h_0+u)^3} \tag{4}$$

where h_0 is the initial gap between the beam and the substrate, and A_{h} is the Hamaker constant. The electrochemical force per unit beam length f_{EC} is the sum of the electrical force per unit beam length f_{E} and chemical (or osmotic) force per unit beam length f_{C}

$$f_{\mathrm{EC}} = f_{\mathrm{E}} + f_{\mathrm{C}} \tag{5}$$

The chemical force is due to the difference in the osmotic pressure of the interstitial solution (P_{i}) and the bulk solution (P_0) with which it is in contact. For a dilute solution

$$f_{\mathrm{C}} = (P_{\mathrm{i}} - P_0)w \tag{6}$$

By combining the general expression for the osmotic pressure of an electrolyte solution and the ionic concentrations c^+ and c^- at equilibrium, one can derive

$$P = kT\sum c_{\mathrm{k}}, \quad c^+ = c_{\mathrm{b}}\exp\left(-\frac{ze\psi}{kT}\right), \quad c^- = c_{\mathrm{b}}\exp\left(\frac{ze\psi}{kT}\right) \tag{7a-c}$$

where c_{b} is the bulk concentration which is assumed to be equal for both ions, e is the electronic charge, z is the absolute value of the valence, ψ is the electric potential, k is the Boltzmann constant, T is the absolute temperature, and we have assumed that the bulk potential is zero. The chemical force can be written as

$$f_{\mathrm{C}} = 2c_{\mathrm{b}}kTw\left[\cosh\left(\frac{ze\psi}{kT}\right) - 1\right] \tag{8}$$

The electric force is

$$f_{\mathrm{E}} = -\frac{1}{2}\varepsilon\varepsilon_0|\nabla\psi|^2 \tag{9}$$

where ε is the relative permittivity of the dielectric medium and ε_0 is the permittivity of free space. The electric potential can be obtained from the Gauss law written in the form of the Poisson–Boltzmann equation given by

$$\nabla^2\psi = -\frac{1}{\varepsilon\varepsilon_0}(zec^+ - zec^-) = \frac{2zec_{\mathrm{b}}}{\varepsilon\varepsilon_0}\sinh\left(\frac{ze\psi}{kT}\right) \tag{10}$$

The Poisson–Boltzmann equation provides accurate results when concentrations do not exceed 1 M and surface potentials are less than 200 mV. For small potentials, the Poisson–Boltzmann equation can be linearized (the Debye–Hückel approximation) to yield

$$\nabla^2\psi = \frac{2z^2e^2c_{\mathrm{b}}}{\varepsilon\varepsilon_0kT}\psi \tag{11}$$

The solution to the linearized Poisson–Boltzmann equation for two parallel plates separated by a distance h with the boundary conditions $\psi(X=0)=\psi_1$ and $\psi(X=h)=\psi_2$ is

$$\psi = \psi_1\cosh(\kappa X) + \frac{\psi_2 - \psi_1\cosh(\kappa h)}{\sinh(\kappa h)}\sinh(\kappa X) \tag{12}$$

The electrochemical force is given by

$$f_{\mathrm{EC}} = w\varepsilon\varepsilon_0\kappa^2\frac{\psi_1^2}{\sinh^2(\kappa h)}\left\{\frac{\psi_2}{\psi_1}\cosh(\kappa h) - \frac{1}{2}\left[1 + \left(\frac{\psi_2}{\psi_1}\right)^2\right]\right\} \tag{13}$$

where $1/\kappa^2 = \varepsilon\varepsilon_0kT/2e^2z^2c_{\mathrm{b}}$, and $1/\kappa$ is the Debye length.

For convenience, the model is written in terms of the non-dimensional variables $h^* = \frac{h}{h_0} = \frac{h_0+u}{h_0}$, $x^* = \frac{x}{L}$ and $\phi = \frac{ze\psi}{kT}$, yielding the following non-dimensional Poisson–Boltzmann equation, equilibrium equation, and forces:

$$\nabla^2\phi = \kappa^2\phi \tag{14}$$

$$\frac{\mathrm{d}^4h^*}{\mathrm{d}x^{*4}} = F_{\mathrm{vdW}} + F_{\mathrm{EC}} \tag{15}$$