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Stochastic surface effects in nanobeam sensors

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ABSTRACT

This work analyzes the statistical properties of nanobeam deflections due to stochastic surface stresses, induced by the surface adsorption/desorption of surrounding particles. A mechanical model for a heterogeneous nanobeam is first introduced. The model considers combined axial forces and bending moments due to non-uniform surface effects. Then, local surface interactions are statistically derived from the Langmuir interaction model and their corresponding stochastic surface stresses are introduced. Two types of nanobeam sensor are studied: a cantilever beam with pure surface bending effect and a clamped beam with mixed surface force and bending moment effects. The advantages of each type are discussed. The deflection statistics are found analytically and validated by Monte Carlo simulations. An analytical relation between the adsorption/desorption rates and the maximum deflection variance is found.

1. Introduction

Microscopic sensors based on deflections of small-scale beams have been developing extensively in recent years. One of their clear advantages is their capability of actuation by surface residual stresses, achieving in situ passive sensing and real-time response.

Surface effects in beams are significant below the microscale. They are introduced by residual stresses and near-surface variations of the elastic modulus [1]. The latter, however, is negligible for sufficiently thick elements [2]. Mechanical modeling of these effects was initiated by Gurtin and Murdoch [3], who formulated the continuum equations and constitutive laws for elastic materials with surface effects. Based on their work, a variety of studies on homogeneous beams and plates were conducted [2,4,5]. Residual stresses of 1D beam models appear on the upper and lower surfaces only. Each surface induces both an axial force and a bending moment on the beam cross section. In axially determinate beams (e.g. cantilever beams) the two effects can be treated separately, while in indeterminate cases (e.g. clamped beams) they are coupled. To our knowledge, only non-coupled cases have been studied so far.

Local variations of surface residual stresses can appear due to interactions with surrounding elements. A variety of interactions are possible: bonding [6,7], partial bonding [8], surface dissociation [9] and surface swelling/collapse [10–12]. Interactions are achieved by coating the surface with a specific receptor layer (surface functionalization).

Surface stress variations cause a spontaneous beam deflection, which was originally used to measure the evolution of surface stresses [13] and later for the actuation of small-scale detectors [14]. These sensors are suitable for detecting a variety of chemical and biological elements such as explosives, pH, DNA, viruses, humidity and more [6,9,15].

In this work we consider the simple but fundamental Langmuir adsorption model, in which interactions occur in specific, immobilized and uncorrelated surface sites [16]. This model is valid for particle adsorption as well as for self-assembly of monolayers on solid surfaces [17,18] and can be used as an initial approximation for more complicated mechanisms. The model predicts the amount of interacting sites without considering their specific locations. Previous studies considered deterministic, uniformly distributed surface stresses, which are proportional to the amount of interacting surface sites. This approach, however, is limited since surface sites are uncorrelated and statistically distributed, leading to non-homogeneous surface stresses.

Microbeam actuators are widely used nowadays. Approaching the nanoscale, surface stochastic heterogeneity is emphasized and a modified analysis is needed. In this work, a mechanical model of a beam with surface heterogeneity is formulated. Inertial effects can be neglected in a typical interaction process ($\sim$1 kHz) [17]. Stochastic effects are estimated analytically by a modified Functional Perturbation Method (FPM) [19,20]. Two nanobeam types are examined: cantilever beams with pure surface bending moment and clamped beams with mixed surface axial force and bending moment. The latter type is less common but its advantages will be demonstrated. Finally, the unique detection benefits of such nanoscale beams are discussed.

2. Mechanical model

In this section the governing equations for nano-Bernoulli beams [2,4,5] are generalized to the case of non-uniform surfaces

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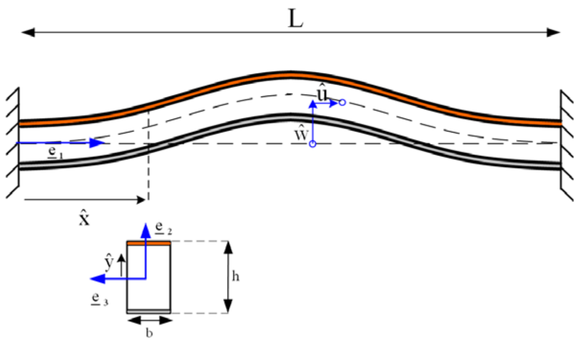

Fig. 1. Schematic description of centerline displacements in a 1D beam.

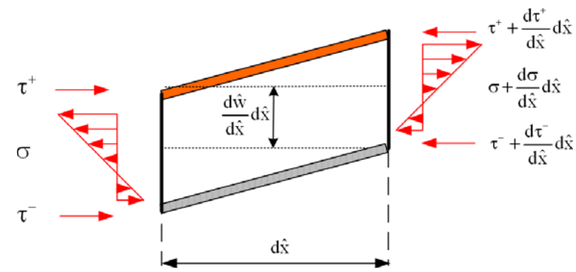

Fig. 2. Free body diagram on a nanobeam segment.

stresses. Consider a beam with length L, height h and breadth b, associated with the in-plane coordinate system $\left(\hat{x},\hat{y}\right)$ and centerline displacements $\left(\hat{u},\hat{w}\right)$, as shown in Fig. 1.

Under Euler–Bernoulli assumptions, the beam displacement field $\left(\tilde{u},\tilde{w}\right)$ refers to the centerline displacements $\left(\hat{u},\hat{w}\right)$ through

$$\tilde{u}=\hat{u}-\hat{y}\frac{\mathrm{d}\hat{w}}{\mathrm{d}\hat{x}} \tag{1}$$

$$\tilde{w}=\hat{w}. \tag{2}$$

For slender beams exhibiting small displacements, the axial strain (ε) is

$$\varepsilon=\frac{\mathrm{d}\tilde{u}}{\mathrm{d}\hat{x}}=\frac{\mathrm{d}\hat{u}}{\mathrm{d}\hat{x}}-\hat{y}\frac{\mathrm{d}^2\hat{w}}{\mathrm{d}\hat{x}^2}. \tag{3}$$

In small-scale beams, the cross section is associated with three normal stress components [4]: the bulk stress σ and two surface residual stresses $\tau^+\delta\left(\hat{y}-\frac{h}{2}\right)$ and $\tau^-\delta\left(\hat{y}+\frac{h}{2}\right)$. δ is a Dirac operator; see the Appendix for further notations. Considering linear elastic materials, σ refers to ε through Young's modulus E:

$$\sigma=E\varepsilon. \tag{4}$$

Under a quasi-static approximation (inertial effects are neglected), force and moment equilibrium on a beam segment associated with first Taylor approximation yields (Fig. 2)

$$b\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left(\tau^++\tau^-\right)-\int\frac{\mathrm{d}\sigma}{\mathrm{d}\hat{x}}b\mathrm{d}\hat{y}=0 \tag{5}$$

$$\int\frac{\mathrm{d}\sigma}{\mathrm{d}\hat{x}}b\hat{y}\mathrm{d}\hat{y}+b\frac{h}{2}\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\left(\tau^--\tau^+\right)-\frac{\mathrm{d}\hat{w}}{\mathrm{d}\hat{x}}\left[b\left(\tau^++\tau^-\right)-\int\sigma b\mathrm{d}y\right]=0. \tag{6}$$

Eqs. (5)–(6) are reduced to the elementary linear beam equations for $\tau^+,\tau^-=0$. Introducing normalized parameters $x=\frac{\hat{x}}{L}$, $u=\frac{\hat{u}}{L}$ and $w=\frac{\hat{w}}{L}$, substituting Eq. (3) into Eq. (4) and then into Eqs. (5)–(6), yields (after some algebra)

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[f_s-a\frac{\mathrm{d}u}{\mathrm{d}x}\right]=0 \tag{7}$$

$$k\frac{\mathrm{d}^4w}{\mathrm{d}x^4}+\frac{\mathrm{d}}{\mathrm{d}x}\left\{\frac{\mathrm{d}w}{\mathrm{d}x}\left[f_s-a\frac{\mathrm{d}u}{\mathrm{d}x}\right]\right\}=\frac{\mathrm{d}^2m_s}{\mathrm{d}x^2}; \tag{8}$$

a, k, f_s and m_s are the cross section axial and bending stiffness, surface force and moment, respectively. In this work a and k are considered constants, while f_s and m_s are generally non-uniform.

$$a=Ehb \tag{9}$$

$$k=E\frac{hb}{12}\left(\frac{h}{L}\right)^2 \tag{10}$$

$$f_s=b\left(\tau^++\tau^-\right) \tag{11}$$

$$m_s=\frac{1}{L}\frac{h}{2}b\left(\tau^--\tau^+\right). \tag{12}$$

Eqs. (7) and (8) govern the centerline displacement field (u,w) for beams without external mechanical loading.

Simplification can be achieved as follows: denote λ^2 as the total cross-sectional force,

$$\lambda^2=f_s-a\frac{\mathrm{d}u}{\mathrm{d}x}. \tag{13}$$

Following Eq. (7), λ^2 is constant and therefore is determined by the axial boundary conditions. Two axial boundary conditions are admissible: fixed edge force (F) or displacements (u_0 and u_1 for $x=0,1$, respectively). Positive values correspond to the positive x direction. For fixed edge force $\lambda^2=-F$, where for predetermined edge displacements λ^2 is found from integration of Eq. (13), i.e.,

$$\lambda^2=\begin{cases}-F & \text{fixed force}\\ \displaystyle\int_0^1 f_s\mathrm{d}x+a\left(u_0-u_1\right) & \text{fixed displacement.}\end{cases} \tag{14}$$

Substituting λ^2 from Eq. (13) into Eq. (8) yields the reduced deflection equation:

$$k\frac{\mathrm{d}^4w}{\mathrm{d}x^4}+\lambda^2\frac{\mathrm{d}^2w}{\mathrm{d}x^2}=\frac{\mathrm{d}^2m_s}{\mathrm{d}x^2}. \tag{15}$$

The four possible boundary conditions for deflection, slope, moment and force, respectively (no external loads), are

$$w=0;\qquad\frac{\mathrm{d}w}{\mathrm{d}x}=0;\qquad k\frac{\mathrm{d}^2w}{\mathrm{d}x^2}=m_s;$$
$$k\frac{\mathrm{d}^3w}{\mathrm{d}x^3}+\lambda^2\frac{\mathrm{d}w}{\mathrm{d}x}=\frac{\mathrm{d}m_s}{\mathrm{d}x}. \tag{16}$$

Eqs. (14)–(15) are the deflection governing equations for beams with non-uniform surface effects. For uniform surface stresses, the right-hand side of Eq. (15) vanishes, and Eq. (14)b is reduced to $\lambda^2=f_s+a\left(u_0-u_1\right)$. When the surface stresses are completely omitted $\left(\tau^+,\tau^-=0\right)$, Eqs. (14)–(15) reduce to the familiar form of the homogeneous case [21].

The present model unifies and generalizes two previous models for pure bending in homogeneous clamped–free beams $\left(m_s=const,\lambda^2=0\right)$ [2,4] and mixed bending (including axial force) in symmetric homogeneous axially fixed beams $\left(m_s=0,\lambda^2=const\right)$ [5].

Two cases are solved here: a cantilever beam in which $\lambda^2=0$ and the right-hand side of Eq. (15) is a stochastic function, representing "pseudo" loading due to surface inhomogeneities, and a clamped–clamped beam which includes also λ^2 as a stochastic functional of the surface heterogeneity.