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# Static bending and vibration analysis of piezoelectric semiconductor beams considering surface effects

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#### Abstract

Based on the surface elasticity theory established by Gurtin and Murdoch, one-dimensional (1D) multi-field coupling model incorporating surface effects for piezoelectric semiconductor (PS) nanostructures is developed, in which the surface effect is treated as a non-classical mechanical boundary condition. With the derived equations, we conduct a theoretical analysis of static bending and free vibration of a simply supported n-type PS beam with open-circuit and electrically isolated boundary conditions at two ends. Numerical results show that the surface effect can stiffen the PS beam, and thus enhance its natural frequencies. Due to the influence of surface effects, the physical quantities such as the effective rigidity and natural frequencies of the PS beam exhibit a considerably significant size-dependent property when the radius R of the PS beam's cross-section is smaller than 400 nm. For the free vibration of the PS beam, the motion of electrons causes a damping effect. Both the surface effect and initial concentration of electrons have an effect on the quasi-damping ratio of the PS beam. The surface effect tends to enhance the damping effect.

Keywords PS beams · Piezotronics · Surface effects · Bending · Vibration

### Introduction

Traditional semiconductors without piezoelectricity such as silicon materials lay the foundation for modern electronics industry and the information age. The third-generation (3G) semiconductors, including ZnO, GaN, and AlN to name but a few, possess both semiconductor properties and piezoelectricity and are also known as piezoelectric semiconductors (PSs). In which the interaction between piezoelectricity and semiconductor behaviors leads to the appearance of piezotronic effects. The key physical mechanism of the

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piezotronic effect is the stress- (or strain) induced polarization acting as a "gate" voltage to adjust the transport behavior of carriers across a PS interface or junction [1–4]. It makes PSs a very promising application in multi-functional sensors and actuators which are crucial to the Internet of Things and Artificial Intelligence age. In recent decades, some researchers have fabricated a lot of low-dimensional PS materials and structures such as one-dimensional (1D) fibers/tubes/belts/spirals, and two-dimensional (2D) filmtype PS structures [5] with good physical and mechanical properties, and used them to make nanogenerators [6–8], field-effect transistors [9, 10], and strain [11, 12]/gas [13, 14]/humidity [15]/chemical [16] sensors.

The prediction of multi-filed coupling behaviors of PSs is of fundamental importance for practical applications of multi-functional PS devices. In recent years, several researchers have conducted insightful theoretical studies on static extension/compression/bending of ZnO rods under different conditions [17–20], free vibration behaviors of ZnO rods [21, 22], and extensional vibrations of ZnO rods [23, 24]. In view of many fiber-based devices [7, 8] usually operating under compression, Liang et al. [25] investigated the static buckling response of a ZnO nanofiber with different boundary conditions with



considering full deformation-polarization-carrier coupling. The analytical expressions of critical forces and stresses, depending on the geometrical aspect, boundary condition, material property, and carrier concentration of the considered PS rod, were presented in Ref. [25], as well. Interestingly, a local load such as a local mechanical force [26] or local temperature change [27] can lead to the formation of local barriers and wells in a single n-type ZnO fiber. This provides a new approach to making an electrical on-off switch device with a single n-/p-type PS structure instead of traditional p-n junction or Schottky contact structures. With the concept of composite material, Cheng et al. [28] and Luo et al. [29] proposed a 2-2 type of laminated PS composite structure consisting of both piezoelectric and semiconductor layers, in which the piezotronic effect is theoretically demonstrated. Furthermore, Cheng et al. [30] realized magnetically controlling of piezotronic effects via a laminated piezomagnetic/PS/ piezomagnetic composite structure. In addition, some researchers have also studied crack problems [31-33] and wave propagation [34–36] in PSs.

For a solid or crystal, the physical properties of the surface are quite different from those of the bulk. However, at macroscopic scale, such a difference brings a very tiny effect to the entire behavior of solids, and is thus negligible. At nanoscale, the surface plays a substantial role in multi-field coupling responses of a solid. For example, Chen et al. [37] experimentally found the size dependence of Young's modulus for ZnO wires, at the same time that for ZnO films was shown in Ref. [38] by atomistic simulations. With the help of the knowledge of differential geometric, Gurtin and Murdoch [39, 40] originally developed a rigorous elastic surface theory within the framework of continuum mechanics, also known as the G-M theory. In the spirit of the G-M theory, a solid includes one three-dimensional (3D) bulk part and the other enclosed two-dimensional material surface part without thickness. Both the surface stress and inertia of the surface part give a traction on the bulk. From the view of equilibrium of the bulk part, the surface effect is identified with a non-classical boundary condition. Based on the G-M theory, researchers have investigated the size-dependent property of macroscopic responses of elastic ultra-thin structures [41, 42], and the influence of surface effects on an isotropic elastic half-space [43]. The G-M theory is also extended to study mechanical behaviors of piezoelectric materials and structures [44–51]. For instance, researchers studied the effect of surface effects on the electromechanical coupling of piezoelectric rings [44] and fibers [48, 49], the buckling behavior [50, 51] of piezoelectric fibers, and on the contact response of a piezoelectric half-plane [45]. A more

generalized structural theory for piezoelectric structures incorporating surface effects was systematically developed in Refs. [46, 47]. It should be mentioned that the nonlocal theory [52, 53] can be also used to investigate macroscopic behaviors of nanostructures.

Similarly, surface effects have to play a significant role in the performance of PS devices at nanoscale. The understanding of how the surface effect influences multi-field coupling behaviors of PS nanostructures is fundamental to the development of PS devices. However, to the authors' knowledge, there is no relevant theoretical study yet. In this paper, based on the G-M theory, we develop the 1D theoretical model for PSs, appropriate to the analysis of PS nanowires/fibers/rods/ beams, by taking the surface effect and full deformationpolarization-carrier coupling into consideration. In doing so, we divide a PS structure into two parts, i.e., of the bulk core and the surface without thickness. The surface effect is treated as the non-classical mechanical boundary condition on the bulk core. With the derived equations, the static bending and free vibration of a simply supported n-type PS beam are investigated. The analytical solutions for displacement, electric potential, and concentration of carriers in the considered PS beam are presented, and the surface effect on the static and free vibration responses are examined as well. The paper is organized as follows. In Sect. 2, the 3D basic equations for PSs and the surface equations for piezoelectric materials are summarized. Based on them, the 1D theoretical model is developed for PSs incorporating surface effects in Sect. 3. Thereupon, the static bending of a simply supported PS beam is studied in Sect. 4, and the free vibration analysis is conducted in Sect. 5. Some numerical results and discussion are provided in Sect. 6. Finally, some conclusions are drawn in Sect. 7.

### **Basic equations**

First briefly summarize the 3D equations of PSs for the bulk part. For a doped PS solid with donors  $N_D^+$  and acceptors  $N_A^-$ , its multi-field coupling behavior can be described by the linear theory of piezoelectricity and semiconductor equations for carriers [54, 55]. The basic physical quantities include displacements  $u_i$ , strains  $S_{ij}$ , stresses  $T_{ij}$ , electric potential  $\varphi$ , electric fields  $E_i$ , electric displacements  $D_i$ , hole and electron concentrations p and n, hole and electron current densities  $J_i^p$  and  $J_i^n$ . The constitutive relations of stresses and electric displacements read

$$T_{ij} = c_{ijkl}S_{kl} - e_{kij}E_k,$$
  

$$D_i = e_{ikl}S_{kl} + \varepsilon_{ik}E_k,$$
(1)

where  $c_{ijkl}$ ,  $e_{kij}$ , and  $\varepsilon_{ij}$  are the elastic, piezoelectric, and dielectric constants, respectively. The strain and electric field components are related to  $u_i$  and  $\varphi$ , respectively

$$S_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \quad E_i = -\varphi_{,i}.$$
 (2)

The hole and electron currents include the drift current the flow of carriers in response to the electric field, and the diffusion current produced by non-uniform distribution of carriers. As the drift current is nonlinear, leading to considerable difficulty in obtaining an analytical solution to the problem, a linearized method is proposed in [19, 56]. In which the hole and electron concentrations are written as  $p = p_0 + \Delta p$  and  $n = n_0 + \Delta n$ , respectively.  $p_0$  and  $n_0$ represent initial concentrations of holes and electrons,  $\Delta p$ and  $\Delta n$  denote perturbations of holes and electrons which are far smaller than p and n, respectively. In this sense, for a uniform-doped PS with  $n_0 = N_D^+$  and  $p_0 = N_A^-$ , the linear constitutive relations of hole and electron current densities can be written as

$$J_i^p = qp_0\mu_{ij}^p E_j - qD_{ij}^p\Delta p_j,$$
  

$$J_i^n = qn_0\mu_{ij}^n E_j + qD_{ij}^n\Delta n_j.$$
(3)

In Eq. (3),  $\mu_{ij}^p$  and  $\mu_{ij}^n$  are the mobility of holes and electrons, and  $D_{ij}^p$  and  $D_{ij}^n$  the diffusion constants of holes and electrons.

For PSs, the equilibrium equations of motion, the charge equation of electrostatics, and the continuity equations for holes and electrons are

$$T_{ij,i} = \rho u_j,$$

$$D_{i,i} = q(\Delta p - \Delta n),$$

$$J_{i,i}^p = -q \frac{\partial}{\partial t} (\Delta p),$$

$$J_{i,i}^n = q \frac{\partial}{\partial t} (\Delta n),$$
(4)

where  $\rho$  is material density, and  $q = 1.6 \times 10^{-19}$ C the elementary charge. It can be seen from Eq. (4) that both piezoelectricity and semiconductor properties are coupled together through the charge equation of electrostatics of Eq. (4)<sub>2</sub>.

For the surface part, according to the G-M theory, the material properties are different from those of the bulk core. The constitute relations of the surface stress components  $T_{ab}^s$  and the electric displacement components  $D_a^s$  at the surface, here *a* and  $b \in (1, 3)$ , are [44]

$$T_{ab}^{s} = T_{ab}^{0} + c_{abcd}^{s} S_{cd} - e_{abk}^{s} E_{k},$$
  

$$D_{a}^{s} = e_{acd}^{s} S_{cd} + e_{ak}^{s} E_{k}.$$
(5)

In Eq. (5),  $T_{ab}^0$  denote the surface residual stress components, and  $c_{abcd}^s$ ,  $e_{abk}^s$ , and  $\varepsilon_{ak}^s$  the surface



Bulk

Fig. 1 Sketch of the G-M surface model

dS

Surface

elastic, piezoelectric, and dielectric constants, respectively. According to the G-M theory, the surface keeps in its equilibrium state under the action of both  $T_{ia}^s$  and  $T_{i2}^{Bs}$ , as shown in Fig. 1. Here,  $T_{i2}^{Bs}$  are the reaction forces of the bulk core against the surface. The surface equilibrium equation reads

$$T_{ia,a}^{s} + T_{i2}^{Bs} = \rho^{s} \ddot{u}_{i}.$$
 (6)

Equation (6) is also referred to as the generalized Young–Laplace equation for curved surfaces or interfaces [57]. Equation (6) can be rewritten as an alternative form of  $T_{i2}^{Bs} = \rho^s \ddot{u}_i - T_{ia,a}^s$ , showing the mechanical nature of the surface effect acting as a non-classical boundary condition. For nanostructures, the surface residual stress also has an effect on their macroscopic behaviors. This mainly depends on the values of the surface residual stress constants  $T_{ab}^0$ , but  $T_{ab}^0$  are difficult to be measured at present. At the same time, our main concern is how the electromechanical coupling of the surface part, which is not included in classical continuum theory, influences macroscopic responses of nanostructures. For convenience, we neglect the effect of the surface residual stress in this paper.

## One-dimensional equations of PS beams incorporating surface effects

In this section, we develop the 1D theoretical model for PSs with surface effects, which are appropriate for investigating common extension/compression/flexural/shear deformations of rod- or beam-like structures. Consider an n-type beam-like PS structure with arbitrary cross-section with a







symmetrical axis as shown in Fig. 2. Its axial line is along with  $x_3$ , and its cross-section locates in the  $x_1-x_2$  plane. Assume that the length of the considered beam is far larger than its transversal aspects.

As stated in the above, we treat the surface effect of PS beams as a non-classical boundary condition. By integrating the product of the 3D field equations and  $x_2$  over the cross-section for the bulk core, the coordinate variables of  $x_1$  and  $x_3$  can thus be canceled out, and then, the 1D theoretical model for PS beams incorporating surface effects can be obtained. According to [54], the zeroth- and first-order equilibrium equations of motion, charge equations of electrostatics, and continuity equations for electrons are

$$T_{aj,a}^{(0)} + \oint_{\Gamma_s} \left[ T_{1j}^{Bs} \right] dx_2 - \oint_{\Gamma_s} \left[ T_{2j}^{Bs} \right] dx_1 = \int_A \rho \ddot{u}_j dA,$$
  
$$T_{aj,a}^{(1)} - T_{2j}^{(0)} + \oint_{\Gamma_s} \left[ x_2 T_{1j}^{Bs} \right] dx_2 - \oint_{\Gamma_s} \left[ x_2 T_{2j}^{Bs} \right] dx_1 = \int_A \rho \ddot{u}_j x_2 dA,$$
  
(7)

$$D_{a,a}^{(0)} + \oint_{\Gamma_s} D_1 dx_2 - \oint_{\Gamma_s} D_2 dx_1 = \int_A q(\Delta p - \Delta n) dA,$$
  
$$D_{a,a}^{(1)} - D_2^{(0)} + \oint_{\Gamma_s} [x_2 D_1] dx_2 - \oint_{\Gamma_s} [x_2 D_2] dx_1 = \int_A q(\Delta p - \Delta n) x_2 dA,$$
  
(8)

$$J_{a,a}^{n(0)} + \oint_{\Gamma_s} J_1^n dx_2 - \oint_{\Gamma_s} J_2^n dx_1 = \int_A q \Delta \dot{n} dA,$$
  
$$J_{a,a}^{n(1)} - J_2^{n(0)} + \oint_{\Gamma_s} [x_2 J_1^n] dx_2 - \oint_{\Gamma_s} [x_2 J_2^n] dx_1 = \int_A q x_2 \Delta \dot{n} dA.$$
  
(9)

 $T_{aj}^{(0)}$ ,  $D_a^{(0)}$ , and  $J_a^{n(0)}$  are the zeroth-order stress, electric displacement, and current density components, respectively, and  $T_{aj}^{(1)}$ ,  $D_a^{(1)}$ , and  $J_a^{n(1)}$  represent the corresponding first-order ones. They are given as

$$T_{aj}^{(0)} = \int_{A} T_{aj} dA, \quad D_{a}^{(0)} = \int_{A} D_{a} dA, \quad J_{a}^{n(0)} = \int_{A} J_{a}^{n} dA,$$
  
$$T_{aj}^{(1)} = \int_{A} x_{2} T_{aj} dA, \quad D_{a}^{(1)} = \int_{A} x_{2} D_{a} dA, \quad J_{a}^{n(1)} = \int_{A} x_{2} J_{a}^{n} dA.$$
  
(10)

It can be seen that Eq. (7) includes the action of the surface part on the bulk core. Substituting  $T_{i2}^{Bs} = \rho^s \ddot{u}_i - T_{ia,a}^s$  into Eq. (7), we can obtain the 1D theoretical model for

PS beams with arbitrary cross-section incorporating surface effects.

Next, we present the 1D basic bending equations for an n-type PS beam with circular cross-section. For the bending PS beam with shear deformation, we assume that the displacements, electric potential, and concentration of incremental electrons have the following approximations [19, 25]:  $u_2 \cong v(x_3, t), u_3 \cong x_2\psi(x_3, t), \varphi \cong x_2\varphi^{(1)}(x_3, t)$ , and  $\Delta n \cong x_2 n^{(1)}(x_3, t)$ . *v* is the deflection,  $\psi$  is the shear deformation accompanying bending. Substituting them into Eqs. (1), (10), and (7), we have

$$Q_{,3}^* = \rho A \ddot{v}, \quad M_{,3}^* - Q^* = \rho I \ddot{\psi},$$
 (11)

where  $Q^* = Q^s + Q$  and  $M^* = M^s + M$ , and

$$M = \overline{c}_{33} I \psi_{,3} + \overline{e}_{33} I \varphi_{,3}^{(1)},$$

$$Q = \overline{c}_{44} A(v_{,3} + \psi) + \overline{e}_{15} A \varphi^{(1)},$$

$$Q^{s} = \left[ c_{44}^{s} \left( v_{,3} + \psi \right) + e_{15}^{s} \varphi^{(1)} \right] \pi R,$$

$$M^{s} = \left( c_{33}^{s} \psi_{,3} + e_{33}^{s} \varphi_{,3}^{(1)} \right) I^{s}.$$
(12)

In Eq. (12),  $I = \pi R^4/4$  is the moment of inertia,  $A = \pi R^2$  the area of the cross-section, and  $I^s = \pi R^3$ . Q and M are the shear force and bending moment of the buck core.  $Q^s$  and  $M^s$  can be regarded as the equivalent shear force and bending moment. From Eqs. (8) and (9), we obtain

$$D_{3,3}^{(1)} - D_2^{(0)} = -qIn^{(1)},$$
  

$$J_{3,3}^{n(1)} - J_2^{n(0)} = qI\dot{n}^{(1)},$$
(13)

where

$$D_{2}^{(0)} = \overline{e}_{15}A(v_{,3} + \psi) - \overline{e}_{11}A\varphi^{(1)},$$
  

$$D_{3}^{(1)} = \overline{e}_{33}I\psi_{,3} - \overline{e}_{33}I\varphi^{(1)}_{,3},$$
(14)

$$J_{2}^{n(0)} = -qn_{0}\mu_{11}^{n}A\phi^{(1)} + qD_{11}^{n}An^{(1)},$$
  

$$J_{3}^{n(1)} = -qn_{0}\mu_{33}^{n}I\phi_{,3}^{(1)} + qD_{33}^{n}In_{,3}^{(1)}.$$
(15)

In Eqs. (12), (14), and (15), the 1D effective material constants are



$$\overline{c}_{33} = 1/s_{33}, \quad \overline{c}_{44} = 1/s_{44}, \quad \overline{e}_{33} = d_{33}/s_{33}, \quad \overline{e}_{15} = d_{15}/s_{44}, \\
\overline{\epsilon}_{11} = \epsilon_{11} - d_{15}^2/s_{44}, \quad \overline{\epsilon}_{33} = \epsilon_{33} - d_{33}^2/s_{33}.$$
(16)

So far, the generalized 1D bending model for PS beams incorporating surface effects is developed, from which the classical Euler–Bernoulli beam model can be obtained by setting the shear strain to zero (namely,  $\psi = -v_{,3}$ ). In doing so, we get the governing equations for bending PS beams without shear deformation

$$-(\overline{c}_{33}I + c_{33}^{s}I^{s})v_{,3333} + (\overline{e}_{33}I + e_{33}^{s}I^{s})\varphi_{,333}^{(1)} = \rho A \ddot{v},$$
  

$$-\overline{e}_{33}Iv_{,333} - \overline{\epsilon}_{33}I\varphi_{,33}^{(1)} + \overline{\epsilon}_{11}A\varphi^{(1)} = -qIn^{(1)},$$
  

$$-n_{0}\mu_{33}^{n}I\varphi_{,33}^{(1)} + D_{33}^{n}In_{,33}^{(1)} + n_{0}\mu_{11}^{n}A\varphi^{(1)} - D_{11}^{n}An^{(1)} = I\dot{n}^{(1)}.$$
(17)

In this case, the equivalent bending moment and shear force, and the resultant electric displacements are

$$M^{*} = -(\overline{c}_{33}I + c_{33}^{s}I^{s})v_{,33} + (\overline{e}_{33}I + e_{33}^{s}I^{s})\varphi_{,3}^{(1)},$$

$$Q^{*} = -(\overline{c}_{33}I + c_{33}^{s}I^{s})v_{,333} + (\overline{e}_{33}I + e_{33}^{s}I^{s})\varphi_{,33}^{(1)},$$

$$D_{2}^{(0)} = -\overline{e}_{11}A\varphi^{(1)},$$

$$D_{3}^{(1)} = -\overline{e}_{33}Iv_{,33} - \overline{e}_{33}I\varphi_{,3}^{(1)}.$$
(18)

# Static bending analysis of PS beams under a uniform distributed load

Consider a simply supported PS beam under static uniform distributed load  $q_0$ . The considered PS beam is with opencircuit and electrically isolated boundary conditions at the two ends. For the static bending of PS beams, the 1D governing equations become

$$-\left(\overline{c}_{33}I + \pi R^3 c_{33}^s\right)v_{,333} + \left(\overline{e}_{33}I + \pi R^3 e_{33}^s\right)\varphi_{,333}^{(1)} = q_0,$$
  

$$-\overline{e}_{33}Iv_{,333} - \overline{e}_{33}I\varphi_{,33}^{(1)} + \overline{e}_{11}A\varphi^{(1)} = -qIn^{(1)},$$
  

$$-n_0\mu_{33}^nI\varphi_{,33}^{(1)} + D_{33}^nIn_{,33}^{(1)} + n_0\mu_{11}^nA\varphi^{(1)} - D_{11}^nAn^{(1)} = 0.$$
(19)

For the simply supported PS beam with open-circuit and electrically isolated boundary conditions at the two ends  $(x_3=0, L)$ , there are

$$v(0) = v(L) = 0,$$
  

$$M(0) = M(L) = 0,$$
  

$$D_3^{(1)}(0) = D_3^{(1)}(L) = 0,$$
  

$$J_3^{n(1)}(0) = J_3^{n(1)}(L) = 0.$$
  
(20)

Equations (19) and (20) constitute a common boundary value problem of partial differential equations. The basic physical quantities v,  $\varphi^{(1)}$ , and  $n^{(1)}$  can be solved as

$$\nu = \frac{f_0}{\beta} \left( C_1 \sinh \beta x_3 + C_2 \cosh \beta x_3 \right) - f_1 \left( \frac{q_0}{24} x_3^4 + \frac{C_0}{6} x_3^3 \right) + C_3 x_3^2 + C_4 x_3 + C_5,$$

$$\varphi^{(1)} = C_1 \cosh \beta x_3 + C_2 \sinh \beta x_3 - f_2 \frac{\overline{e}_{33}}{q \overline{e}_{33}} \left( C_0 + q_0 x_3 \right),$$

$$n^{(1)} = \frac{n_0 q}{kT} \varphi^{(1)}.$$

$$(21)$$

In Eq. (21)

$$\begin{split} C_{0} &= -\frac{q_{0}L}{2}, \ C_{1} = 2\frac{(1-\cosh\beta L)}{\beta\sinh\beta L}\frac{\overline{e}_{33}}{\overline{e}_{33}}f_{2}, \\ C_{2} &= \frac{\overline{e}_{33}f_{2}}{\overline{e}_{33}}, \ C_{3} = \frac{f_{2}f_{0}}{2}\frac{\overline{e}_{33}}{\overline{e}_{33}}, \\ C_{4} &= -f_{0}f_{2}\frac{\overline{e}_{33}}{\overline{e}_{33}}\left(\frac{1-\cosh\beta L}{\beta^{2}L} + \frac{L}{2}\right) - \frac{q_{0}f_{3}L^{3}}{24}, \ C_{5} = -\frac{f_{0}f_{2}}{\lambda_{3}^{2}}\frac{\overline{e}_{33}}{\overline{e}_{33}}, \\ f_{0} &= \frac{\overline{e}_{33}I + e_{33}^{s}I^{s}}{\overline{c}_{33}I + e_{33}^{s}I^{s}}, \ f_{1} &= \frac{1}{\overline{c}_{33}I + e_{33}^{s}I^{s}}, \\ f_{2} &= \frac{\overline{e}_{33}q_{0}}{\left(\overline{e}_{11}\frac{A}{I} + \frac{n_{0}q^{2}}{kT}\right)\left(\overline{c}_{33} + e_{33}^{s}I^{s}/I\right)}, \ \beta &= \sqrt{\left(\overline{e}_{11}\frac{A}{I} + \frac{n_{0}q^{2}}{kT}\right)\left/\left(\overline{e}_{33}f_{0} + \overline{e}_{33}\right)} \end{split}$$



In addition, from Eq. (19) we can obtain the effective flexural rigidity of  $[EI]_s = \left(\overline{c}_{33} + \frac{\overline{e}_{33}^2}{\overline{c}_{33}}\right)I + \left(c_{33}^s + \frac{\overline{e}_{33}e_{33}^s}{\overline{c}_{33}}\right)I^s$  of the considered PS beam through writing the bending equation in terms of the deflection v. The first term  $\left(\overline{c}_{33} + \frac{\overline{e}_{33}^2}{\overline{e}_{33}}\right)I$  denoted by  $[EI]_0$  represents the classical flexural rigidity of PS beams without considering surface effects. The second term resulting from the surface part plays a dominant role at nanoscale, while is negligible at macroscale.

# Free bending vibration of a simply supported PS beam

In this section, consider the free bending vibration of a simply supported PS beam. Strictly speaking, it is a damped free vibration resulting from the motion of carriers. Assume the following solutions [25], satisfying with the boundary conditions of Eq. (20), as

$$v = A_1 \sin k_m x_3 q(t),$$
  

$$\varphi^{(1)} = A_2 \cos k_m x_3 q(t),$$
  

$$n^{(1)} = A_3 \cos k_m x_3 q(t),$$
  
(22)

where  $A_1$ ,  $A_2$ , and  $A_3$  are unknown constants,  $k_m = m\pi/L$ (m=1, 2, 3...),  $q(t) = \exp(\lambda t)$  reflects the oscillation behavior of the considered PS beam. The substitution of Eq. (22) into Eq. (17), yields

$$\begin{aligned} a_{0} &= \rho \frac{1}{c} \left( \frac{k_{m}^{2} \overline{\epsilon}_{33}}{c} + \overline{\epsilon}_{11} \right), c = A/I, \\ a_{1} &= \rho \left( \frac{k_{m}^{2} \overline{\epsilon}_{33}}{c} + \overline{\epsilon}_{11} + \frac{q n_{0} \mu_{33}^{n}}{c D_{33}^{n}} \right) \left( \frac{k_{m}^{2} D_{33}^{n}}{c} + D_{11}^{n} \right), \\ a_{2} &= \overline{e}_{33} \left( \overline{e}_{33} + \frac{4 e_{33}^{s}}{R} \right) \frac{k_{m}^{6}}{c^{3}} + \left( \frac{k_{m}^{2} \overline{\epsilon}_{33}}{c} + \overline{\epsilon}_{11} \right) \left( \overline{c}_{33} + \frac{4 c_{33}^{s}}{R} \right) \frac{k_{m}^{4}}{c^{2}}, \\ a_{3} &= \overline{e}_{33} \left( \overline{e}_{33} + \frac{4 e_{33}^{s}}{R} \right) \left( \frac{k_{m}^{2} D_{33}^{n}}{c} + D_{11}^{n} \right) \frac{k_{m}^{6}}{c^{2}} \\ &+ \left( \frac{k_{m}^{2} \overline{\epsilon}_{33}}{c} + \overline{\epsilon}_{11} + \frac{q n_{0} \mu_{33}^{n}}{c D_{33}^{n}} \right) \left( \overline{c}_{33} + \frac{4 c_{33}^{s}}{R} \right) \left( \frac{k_{m}^{2} D_{33}^{n}}{c} + D_{11}^{n} \right) \frac{k_{m}^{4}}{c}. \end{aligned}$$

$$(25)$$

In Eq. (25),  $a_1$  and  $a_3$  contain material constants related to semiconductor properties, while  $a_0$  and  $a_2$  do not. For the case of pure piezoelectric beams, both  $a_1$  and  $a_3$  are zeros in Eq. (25), and thus, the characteristic equation of Eq. (24) becomes

$$\left(a_0\lambda^2 + a_2\right)\lambda = 0. \tag{26}$$

We immediately have

$$\lambda_1 = 0, \ \lambda_{2,3} = \pm i \sqrt{a_2/a_0}.$$
 (27)

The zero root  $\lambda_1$  has no physical meaning and is thus omitted. Accordingly, the general solution of q(t) is

$$q(t) = B_1 \cos \omega_m t + B_2 \sin \omega_m t.$$
<sup>(28)</sup>

$$\begin{bmatrix} \overline{e}_{33}k_m^3 & \overline{e}_{33}k_m^2 + \overline{e}_{11}c & q \\ 0 & n_0(\mu_{33}^n k_m^2 + \mu_{11}^n c) & -(D_{33}^n k_m^2 + D_{11}^n c + \lambda) \\ -(\overline{c}_{33} + c_{33}^s cR)k_m^4 - \rho c \lambda^2 & (\overline{e}_{33} + cRe_{33}^s)k_m^3 & 0 \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$
(23)

The existence of a nontrivial solution requires that the determinant of coefficient matrix of Eq. (23) must be zero. This yields the following characteristic equation:

$$a_0\lambda^3 + a_1\lambda^2 + a_2\lambda + a_3 = 0, (24)$$

where

$$B_1$$
 and  $B_2$  are unknown constants and dependent on the initial condition. The *m*th-order natural frequency  $\omega_m$  is given as

$$\omega_{m} = \operatorname{Im}[\lambda_{2}] = \sqrt{a_{2}/a_{0}} = k_{m}^{2} \sqrt{\frac{1}{\rho c}} \sqrt{\overline{c}_{33} + \frac{4c_{33}^{s}}{R} + \frac{\overline{e}_{33}(\overline{e}_{33} + 4e_{33}^{s}/R)}{\overline{e}_{33} + c\overline{e}_{11}/k_{m}^{2}}}.$$
(29)

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In Eq. (29), by getting rid of corresponding material constants, we can directly obtain the natural frequencies for piezoelectric  $({}^{s}\omega_{m}^{PE})$  and pure elastic  $({}^{s}\omega_{m}^{E})$  beams with considering surface effects, and those for piezoelectric  $(\omega_{m}^{PE})$  and pure elastic beams  $(\omega_{m}^{E})$  beams without considering surface effects. They are

$${}^{s}\omega_{m}^{PE} = {}^{s}\omega_{m}^{E}\sqrt{1 + {}^{s}\overline{k}_{33}^{2}\left(1 + \frac{c\overline{\epsilon}_{11}}{\overline{\epsilon}_{33}k_{m}^{2}}\right)^{-1}}, \quad {}^{s}\omega_{m}^{E} = \omega_{m}^{E}\sqrt{1 + \frac{4c_{33}^{s}}{\overline{c}_{33}R}},$$
$$\omega_{m}^{PE} = \omega_{m}^{E}\sqrt{1 + \overline{k}_{33}^{2}\left(1 + \frac{c\overline{\epsilon}_{11}}{\overline{\epsilon}_{33}k_{m}^{2}}\right)^{-1}}, \qquad \omega_{m}^{E} = k_{m}^{2}\sqrt{\frac{\overline{c}_{33}}{c\rho}}.$$
(30)

In Eq. (30), 
$${}^{s}\bar{k}_{33} = \bar{k}_{33}\sqrt{\left(1 + \frac{4e_{33}^{s}}{\bar{e}_{33}R}\right)\left(1 + \frac{4e_{33}^{s}}{\bar{e}_{33}R}\right)^{-1}}$$
 and

 $\bar{k}_{33} = \sqrt{\frac{e_{33}}{\bar{c}_{33}\bar{e}_{33}}}$  represent the electromechanical coupling coefficients of piezoelectric beams with and without considering surface effects. Equation (30) implies that both piezoelectricity and surface effects tend to increase the natural frequencies of structures. This is because they increase the effective flexural rigidity of PS beams. Note that the surface effect maybe increases or decreases natural frequencies of PS beams when considering surface positive or negative residual stresses.

Next, we solve the characteristic equation [Eq. (24)] for PS beams. The motion of carriers inside PSs plays a fundamental role in semiconductor devices. However, the motion of carriers can cause a damping effect in the bending vibration of PS beams at the same time. The three roots  $(\lambda_1, \lambda_2, \text{ and } \lambda_3)$  of the characteristic equation Eq. (24) can be obtained in terms of Cardan's formula

$$\lambda_{1} = -\frac{a_{1}}{3a_{0}} + Y_{1}^{\frac{1}{3}} + Y_{2}^{\frac{1}{3}},$$

$$\lambda_{2,3} = -\frac{a_{1}}{3a_{0}} - \frac{1}{2}(Y_{1}^{\frac{1}{3}} + Y_{2}^{\frac{1}{3}}) \pm i\frac{\sqrt{3}}{2}(Y_{1}^{\frac{1}{3}} - Y_{2}^{\frac{1}{3}}),$$
(31)

where  $Y_{1,2} = -\frac{p_2}{2} \pm \sqrt{\left(\frac{p_2}{2}\right)^2 + \left(\frac{p_1}{3}\right)^3}$ ,  $p_1 = \frac{3a_0a_2 - a_1^2}{3a_0^2}$ , and  $p_2 = \frac{27a_0^2a_3 - 9a_0a_1a_2 + 2a_1^3}{27a_0^3}$ . When  $\Delta = \left(\frac{p_2}{2}\right)^2 + \left(\frac{p_1}{3}\right)^3$  is positive, there are one real root  $\lambda_1$  and two complex conjugate roots  $\lambda_{2,3}$ . For the considered PS beam in this paper,  $\Delta$  is always positive, which is numerically shown in **Appendix I**. In this case, the oscillation motion q(t) can be written as in the form of

$$q(t) = B_1 e^{-\zeta_{1m}\omega_m t} + e^{-\zeta_{2m}\omega_m t} (B_2 \cos \omega_m^d t + B_3 \sin \omega_m^d t).$$
(32)

In Eq. (32), there are  $\zeta_{1m} = -\lambda_1/\omega_m$  and  $\zeta_{2m} = -\text{Re}[\lambda_2]/\omega_m$ , the expression of  $\omega_m$  has been given as  ${}^s\omega_m^{PE}$ in Eq. (30).  $\omega_m^d = \text{Im}[\lambda_2] = \frac{\sqrt{3}}{2}(Y_1^{\frac{1}{3}} - Y_2^{\frac{1}{3}})$  represents natural frequencies of damped free bending vibration of PS beams. In Eq. (32), both  $e^{-\zeta_{1m}\omega_m t}$  and  $e^{-\zeta_{2m}\omega_m t}$  are exponentially decaying functions of time. The first term  $B_1 e^{-\zeta_{1m}\omega_m t}$ indicates a rapidly decaying motion without oscillation corresponding to the overdamped case of classical vibration theory [56]. For the considered problem,  $\zeta_{1m}$  is far larger than  $\zeta_{2m}$  which can be shown in Fig. 11 (see Sect. 6). Actually, it is not possible that the motion of carriers produces such a "huge" damping effect in the free bending vibration of PS beams. Hence,  $B_1 e^{-\zeta_{1m}\omega_m t}$  should be deleted, namely, we have

$$q(t) = e^{-\zeta_{2m}\omega_m t} \left( B_2 \cos \omega_m^d t + B_3 \sin \omega_m^d t \right).$$
(33)

The two unknown constants  $B_2$  and  $B_3$  can be determined from initial conditions. To make a representation of q(t), without loss generality, we assume initial conditions with  $q(0) = Q_0$  and  $\dot{q}(0) = Q_1$ . Substituting them into Eq. (33), we get  $B_2 = Q_0$  and  $B_3 = (\zeta_{2m}\omega_m Q_0 + Q_1)/\omega_m^d$ , and then

$$q(t) = \sqrt{B_2^2 + B_3^2} e^{-\zeta_{2m}\omega_m t} \sin\left(\omega_m^d t + \Phi\right),$$
 (34)

where  $\Phi = \arctan \left[ Q_0 \omega_m^d / (\zeta_{2m} \omega_m Q_0 + Q_1) \right]$ . Following the similar approach as in Ref. [58], we can evaluate the rate of decay of free oscillations of PS beams through computing the natural logarithm of the ratio of any two successive amplitudes, that is

$$\delta = \ln \frac{q(t_1)}{q(t_1 + \tau_d)} = \zeta_{2m} \omega_m \tau_d.$$
(35)

 $\tau_d = 2\pi/\omega_m^d$  is the damped period. In addition, we define the decay time  $t_{decay}$  as the period of the amplitude



**Fig. 3** Normalized effective flexural rigidity  $[EI]_s/[EI]_0 = 1 + 4$  $\frac{h_0}{R} \frac{c_{33}\tilde{\epsilon}_{33} + \tilde{\epsilon}_{33}^2}{\tilde{\epsilon}_{33}\tilde{\epsilon}_{33} + \tilde{\epsilon}_{33}^2}$ 



**Fig. 4** Distributions of electromechanical fields at  $x_2 = R$ : **a** deflection  $\blacktriangleright$  *v*, **b** potential  $\varphi$ , **c** incremental carrier concentrations  $\Delta n$  (L=600 nm, R=30 nm,  $n_0=10^{23}$  m<sup>-3</sup>)

 $\sqrt{Q_0^2 + Q_1^2 e^{-\zeta_{2m}\omega_m t}}$  decaying by a factor of 1/e. Then, we have

$$t_{decay} = 1/\zeta_{2m}\omega_m. \tag{36}$$

### Numerical examples and discussion

In this section, we use the derived theoretical model to numerically study the static bending and free vibration of a simply supported beam made of n-type ZnO. As numerical examples, the length of the beam and the radius of crosssection are chosen as L=600 nm and R=30 nm, and the initial electron concentration is  $n_0 = 10^{23}$  m<sup>-3</sup>. The materials constants of the bulk ZnO are from Ref. [55]. For the sake of simplicity, we adopt the same feasible and reasonable method as in Ref. [47] for the surface material constants  $f_S$ , that is, they are proportional to its bulk counterpart  $f_B$ . The scale factor is equivalent to the intrinsic material length  $h_0$ . Namely,  $f_S \approx f_B h_0$ . According to Ref. [59], the intrinsic material length of ZnO is chosen as  $h_0=0.4$  nm in this paper.

First, consider the static bending of the PS beam under different uniform distributed forces ( $q_0 = 0.5$ , 1.0, and  $2 \times 10^{-2}$  N/m) per unit width. With the analytical solutions obtained in Sect. 4, we can evaluate the effective flexural rigidity  $[EI]_{c}$ , deflection v, electric potential  $\varphi$ , and incremental concentration of electrons  $\Delta n$  along the PS beam. Figure 3 shows the size-dependent characteristics of  $[EI]_s$ normalized by  $[EI]_0$ . It can be observed that the surface effect almost has no effect when  $R/h_0$  is greater than 100 or so (namely, the radius of the beam is larger than about 400 nm); however, it brings a dramatic change of the effective flexural rigidity  $[EI]_s$  when R is smaller than 400 nm. For example,  $[EI]_s$  increases from  $1.1[EI]_0$  to  $1.6[EI]_0$  with R decreasing from 400 to 40 nm. Such a phenomenon attributed to the surface effect can be called the surface-induced stiffening effect, similar to the piezoelectric stiffening effect.

Figures 4 shows the distribution of  $\nu$ ,  $\varphi = R\varphi^{(1)}$ , and  $\Delta n = Rn^{(1)}$  along the beam at  $x_2 = R$  without/with considering surface effects. It can be observed that for the considered PS beam, the surface effect plays a decreasing role in the mechanical and electrical responses of the PS beam due to the surface-induced stiffening effect. For example, the surface effect lowers the amplitude of  $\nu$ ,  $\varphi$ , and  $\Delta n$ . The electrical potential displays an almost linear and anti-symmetric distribution along its axial direction ( $x_3$ ) of the PS beam, as shown in Fig. 4b. It can be seen, from Fig. 4c that the









R = 30 nm)





Fig. 6 The 1st-order normalized natural frequencies under different values of  $R/h_0$  with L/R = 20

distribution of  $\Delta n$  exhibits the same trend as the electric potential. This is because of the electrons redistributing itself driven by the induced piezoelectric potential. The electrons have a larger variation in the two ends.

Next, consider the free bending vibration of the PS beam with the same geometrical size as it in the preceding example. Based on the analytical expressions derived in Sect. 5, we set m = 1 to evaluate the first-order natural frequencies of the PS beam under different initial concentrations. Meanwhile, the first-order natural frequencies for piezoelectric and elastic beams with the same geometrical size are also provided. These frequencies normalized by  $\omega_1^E$ are plotted in Fig. 5. The symbols of 'PS', 'PE', and 'Elastic' appeared in Figs. 5 and 6 denote the cases of piezoelectric semiconductor, piezoelectric, and elastic beam, respectively. From Fig. 5, we find that the surface effect makes the natural frequencies a significant increase. For different initial electron concentrations  $n_0$ , the first-order natural frequencies of the PS beam are always larger than those of pure elastic beams, while are smaller than ones of piezoelectric beams. Only the initial concentration of electrons ranging from  $10^{22}$  $m^{-3}$  to  $10^{24} m^{-3}$  plays a tuning role in the natural frequencies of PS beams.

To get a deeper understanding of size-dependent properties of the considered bending PS beam due to surface effects, we calculate the first-order natural frequencies for different values of  $R/h_0$  when  $n_0 = 10^{23} \text{ m}^{-3}$ , the ratio of L/R = 20, and  $h_0 = 0.4$  nm are fixed. Figure 6 shows the size-dependent property of the 1st-order natural frequency of the PS beam. With the reduction of R, the surface effect makes the first-order natural frequency a dramatic rise. This









is because of the surface-induced stiffening effect. The surface effect should be taken into consideration when the value of  $R/h_0$  decreases to about 400 for the considered PS beam.

It is the motion of carriers that produces a damping force for the vibration of PS beams. Such a damping effect mainly depends on the total amount of carriers. We compute the quasi-damping ratio  $\zeta_2$  for different initial concentrations of electrons, and the value of  $\zeta_1$  is also evaluated. The curves of  $\zeta_1$  and  $\zeta_2$  under different initial concentrations of electrons are plotted in Fig. 7. It can be observed from Fig. 7 that  $\zeta_1$  is more than 10 orders of magnitude larger than  $\zeta_2$ . Figure 7b shows the quasi-damping ratio  $\zeta_2$  increases from zero to its maximum 7.15 × 10<sup>-8</sup> with  $n_0$  increasing to about 8 × 10<sup>22</sup> m<sup>-3</sup>, and then,  $\zeta_2$  decreases sharply with the increase of  $n_0$ . The quasi-damping ratio  $\zeta_2$  with surface effects is larger than those without surface effects.

Figure 8 shows the decay behavior of the oscillatory amplitude of q(t) for different initial concentrations of electrons without and with considering surface effects. The initial concentration of electrons has an important effect on the decaying of the oscillatory amplitude of q(t). This is because the value of quasi-damping ratio  $\zeta_2$  is dependent

on the initial concentration of electrons. To represent the dependent relation of the decay time on the initial concentration of electrons in detail, we plot the decay time and the normalized decay time by  $2\pi/\omega_d$  under different initial concentrations of electrons in Fig. 9. It can be seen that the considered PS beam undergoes a faster-attenuating oscillation when  $n_0 \in (10^{22}, 10^{24})$ .

### Conclusions

In summary, based on the G-M surface theory, we treat the surface effect as a non-classical boundary condition and develop the 1D deformation-polarization-carrier coupling model for beam-like PS nanostructures with arbitrary cross-section. The derived equations are useful for studying the bending of PS beams at nanoscale. Both the static bending and free vibration analysis of a simply supported n-type PS beam with open circuit and electrically isolated boundary conditions are investigated. For the static bending of the PS beam under the uniform distributed load  $q_0$ , the analytical solutions of the effective flexural rigidity, deflection,

potential, and incremental concentration of electrons are presented. For the free vibration of the PS beam, the analytical expressions of natural frequencies and the carriers-induced damping effect are presented. Such a damping effect due to the motion of carriers depends on the initial concentration of electrons. The initial concentration of electrons ranging from  $10^{22}$  m<sup>-3</sup> to  $10^{24}$  m<sup>-3</sup> leads to a strong damping effect. The surface effect has a remarkable effect on the effective flexural rigidity and natural frequencies of the bending PS beam. The initial concentration of electrons plays a role in the natural frequencies and oscillation motion of the bending PS beam. The numerical results are helpful to understand multi-field coupling behaviors of PS nanostructures, and in designing PS nanodevices, as well.

### Appendix I: Numerical values of $\Delta$

In Eq. (31), the three roots  $\lambda_1$ ,  $\lambda_2$ , and  $\lambda_3$  are available when

$$\Delta = \left(\frac{p_2}{2}\right)^2 + \left(\frac{p_1}{3}\right)^3 > 0.$$
 (A1)

The material and geometrical constants of the ZnO PS beam have been given in Sect. 6. We evaluate  $\Delta$  under different initial concentrations of electrons and plot it in Fig. 10. It can be seen that  $\Delta$  is always positive and has a very large value.



Fig. 10  $\Delta$  in Eq. (A1) for different initial concentrations of electrons. (*L*=600 nm, *R*=30 nm)

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