Static buckling of piezoelectric semiconductor fibers

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Abstract
We develop a one-dimensional static buckling model for piezoelectric semiconductor fibers with taking the coupling of deformation, polarization, and carriers into consideration based on the macroscopic theory of piezoelectric semiconductors. The obtained buckling model is an extension of classical elastic and piezoelectric ones. The buckling of piezoelectric semiconductor fibers under axial forces is studied with the proposed one-dimensional buckling model. An exact solution for a simply-supported fiber is obtained from the model, which shows the basic physics involved explicitly. The result for a simply-supported fiber is extended to fibers with other end supports using the concept of effective length from the mechanics of materials, and to fiber arrays which are widely used in devices.

1. Introduction

Piezoelectric crystals are either dielectrics or semiconductors. This paper is concerned with the latter in which multiple electromechanical fields including deformation, polarization, and semiconduction can co-exist. These fields also interact through a series of coupling effects. When piezoelectric semiconductors are under mechanical loads, stress or strain develops and causes electric polarization through piezoelectric coupling. The electric field associated with the polarization then drives the holes and electrons, producing electric currents or redistributions of charge carriers. The mobile charges also screen the polarization and weaken the piezoelectric coupling. Piezoelectric semiconductors have been used to make acoustoelectric devices for charge transport and acoustic wave amplification for quite some time [1]. During the past one to two decades, various new piezoelectric semiconductor structures have been synthesized such as zinc oxide (ZnO) and molybdenum disulfide (MoS₂) fibers, tubes, belts, spirals, and films. These relatively new structures have led to new applications of piezoelectric semiconductors in sensing and transduction, optoelectronics, electro- and photochemical processes, nanogenerators, electronics and phototronics. The studies on the interactions between mechanical fields and mobile charges at PN junctions and MS (metal-semiconductor) junctions have formed new research areas called piezotronics and piezo-phototronics [2–3].

Many piezoelectric semiconductor devices are based on single fibers [3, 6] or fiber arrays [7–11]. These fibers may be in extension, compression, or bending. While there exist extensive studies on the extension [12–18] and bending [19–24] of fibers, an important phenomenon associated with fibers in compression, i.e., the buckling of a piezoelectric semiconductor fiber or fiber arrays seems to have been missing by the literature. Compressive loads are common in devices made from fiber arrays between two films [7–10]. Analysis of buckling and instability of a compressed rod- or wire-structures is crucial in designing of devices. Some researchers have investigated the buckling of ZnO or other elastic structures [25–27]. For example, Riaz et al. [28] studied the buckling of vertical ZnO rods. Wang et al. [27] investigated the buckling behavior of compressed ZnO nanowires using MD simulations. However, the existed theoretical buckling models are only suitable for elastic and piezoelectric structures. They cannot be used to treat the buckling behavior of piezoelectric semiconductor
structures due to not incorporating semiconducting property. To develop piezoelectric semiconductor devices with good performance and high reliability, it is of fundamental importance that to investigate the buckling of a piezoelectric semiconductor fiber by taking the fully coupling of carrier, deformation and polarization. In this paper, we present a theoretical buckling model of piezoelectric semiconductor fibers and analyze the buckling behaviors of piezoelectric semiconductor fibers. In addition, we also extend the results obtained for a single fiber to fiber arrays.

2. One-dimensional equations for bending of a fiber

Consider an n-type ZnO fiber with a circular cross section as shown in figure 1. Let the concentration of the donor impurity be \(N_D^0\) which is a constant for the case of uniform doping we are considering. For simplicity, we denote \(n_0 = N_D^0\) which is the electron concentration at the reference state before buckling. When the fiber buckles, we write the current electron concentration by \(n = n_0 + \Delta n\) where \(\Delta n\) is the electron concentration perturbation due to buckling.

The basic behaviors of piezoelectric semiconductors can be described by a macroscopic theory which consists of the conventional theory of piezoelectricity for dielectrics [28] and the drift-diffusion theory of semiconductors [29]. For piezoelectric semiconductors, the two theories are coupled by the doping and mobile charges in the charge equation of electrostatics [12]. Such a coupled theory has been used in the literature to study various problems in piezoelectric semiconductors including extension [12–18] and bending [19–24] of fibers, waves and vibrations [30–37], cracks [38–43], and fields near PN junctions [13].

For the bending of piezoelectric semiconductor fibers, a set of one-dimensional (1-D) linear equations was derived in [22] from the general three-dimensional (3D) coupled-fields theory. It should be noted that the linearized method is employed for the case of small carrier concentration perturbation in [22]. We still consider this situation in this paper. In the 1D model, the relevant mechanical displacements \(u_2\) and \(u_3\), electrical potential \(\varphi\), and electron concentration perturbation \(\Delta n\) relevant to buckling or bending in the \(x_3-x_2\) plane are approximated by [22, 23]:

\[
\begin{align*}
  u_2 &\approx v(x_3, t), \\
  u_3 &\approx x_2 \psi(x_3, t), \\
  \varphi &\approx x_2 \phi^{(1)}(x_3, t), \\
  \Delta n &\approx x_2 n^{(1)}(x_3, t),
\end{align*}
\]

where \(v(x_3, t)\) is the bending displacement or the deflection, and \(\psi(x_3, t)\) the shear deformation accompanying bending. The 1D bending theory is a moment-type theory involving the zero- and first-order moments of the relevant fields. The 1D equations of motion, charge equation of electrostatics, and conservation of charge for electrons are obtained by integrating the corresponding 3D field equations and their products with \(x_2\) over the fiber cross section. When the lateral surface of the fiber is free of traction, charge and currents, the 1D field equations are [22, 23]

\[
\begin{align*}
  Q_{3,3} &= \rho A_i \ddot{v}, \\
  M_{3,3} - Q &= \rho l \ddot{\psi}, \\
  D_{3,3}^{(1)} - D_2^{(0)} &= qI(-n^{(1)}), \\
  f_{3,3}^{(1)} - f_2^{(0)} &= qH^{(1)},
\end{align*}
\]

where \(Q\) is the transverse shear force, \(M_i\) the bending moment, \(\rho\) the mass density, \(q\) the elementary charge. \(D_2^{(0)}, D_2^{(1)}, f_2^{(0)}\) and \(f_2^{(1)}\) are the zeroth- and first-order moments of the relevant electric displacement components and current components. \(A_i\) is the total area of the cross section of the fiber and \(I\) is the moment of inertia of the cross section with respect to the \(x_3\) axis. Equation (2) is the equilibrium equation of stress in the \(x_2\) (or \(y\)) direction, equation (2) is the equilibrium equation of moment about the axis of \(x_3\), equation (2) is the electrostatic charge equation, and equation (2) is the continuity equation of charge. For a circular cross-section
fiber with radius \( r = a \), there are

\[
I = \int_A x^2 \, dA = \frac{\pi a^4}{4}, \quad A_r = \pi a^2.
\]

The expressions of \( M_1, Q, D_2^{(0)}, D_3^{(1)}, J_2^{(0)} \) and \( J_3^{(1)} \) in equation (2) are [22, 23]

\[
M_1 = \int_A x_1 T_1 \, dA = \varepsilon_{33} I_{v,3} + \varepsilon_{31} I_{\phi,3}^{(1)},
\]

\[
Q = \int_A T_1 \, dA = \varepsilon_{44} A_r (v,3 + \psi) + \varepsilon_{33} A_r \phi^{(1)},
\]

\[
D_2^{(0)} = \int_A D_2 \, dA = \varepsilon_{33} A_r (v,3 + \psi) - \varepsilon_{11} A_r \phi^{(1)},
\]

\[
D_3^{(1)} = \int_A x_2 D_3 \, dA = \varepsilon_{33} I_{v,3} - \varepsilon_{33} I_{\phi,3}^{(1)},
\]

\[
J_2^{(0)} = \int_A J_2^s \, dA = -q n_0 \mu_1^n A_r \phi^{(1)} + q D_4^{(0)} A_r n^{(1)},
\]

\[
J_3^{(1)} = \int_A x_2 J_3^s \, dA = -q n_0 \mu_3^n A_r I_{\phi,3}^{(1)} + q D_5^{(0)} n_{\phi,3}^{(1)},
\]

where the 1D effective material constants for thin fibers are [22]

\[
\varepsilon_{33} = 1/s_{33}, \quad \varepsilon_{44} = 1/s_{44}, \quad \varepsilon_{33} = d_{33}/s_{33}, \quad \varepsilon_{33} = d_{15}/s_{44},
\]

\[
\varepsilon_{11} = \varepsilon_{11} - d_{15}^2/s_{44}, \quad \varepsilon_{33} - d_{33}^2/s_{33}.
\]

In equations (6) and (7), \( s_{33} \) are the elastic compliance, \( d_{33} \) the piezoelectric constant, \( \varepsilon_{33} \) the dielectric constant, \( \mu_0^n \) the electron mobility, and \( D_4^n \) the hole diffusion constant in the matrix notation reduced from the tensor notation [28]. The appearance of the effective 1D material constants in equations (4) and (3) is because of the use of the following usual stress relaxation approximation for thin fibers:

\[
T_1 \cong 0, \quad T_2 \cong 0.
\]

The above equations are for bending with shear deformation. For the purpose of this paper, it is sufficient to consider a special case of the above theory, i.e., bending without shear deformation which is the common-used Euler–Bernoulli beam theory. To reduce the above equations to the Euler–Bernoulli beam model, we set the fiber shear strain \( v,3 + \psi \) to zero, which implies that

\[
\psi = -v,3.
\]

Then equations (4), and (5) reduce to

\[
M_1 = -\varepsilon_{33} I_{v,33} + \varepsilon_{31} I_{\phi,33}^{(1)},
\]

\[
D_2^{(0)} = -\varepsilon_{11} A_r \phi^{(1)},
\]

\[
D_3^{(1)} = -\varepsilon_{33} I_{v,33} - \varepsilon_{33} I_{\phi,33}^{(1)},
\]

In the theory of bending without shear deformation, the moment of inertia on the right-hand side of equation (2)_2 can be neglected. Then equation (2)_2 implies that

\[
Q = M_1,3 = -\varepsilon_{33} I_{v,333} + \varepsilon_{33} I_{\phi,333}^{(1)} = \rho A_r \ddot{y}.
\]

where equation (10) has been used. Effectively, equation (12) serves as the constitutive relation for \( Q \) which, when substituted into equation (2)_1, yields the following equation for bending without shear deformation:

\[
-\varepsilon_{33} I_{v,333} + \varepsilon_{33} I_{\phi,333}^{(1)} = \rho A_r \ddot{y}.
\]

The substitution of equation (11) into equation (2)_3 yields

\[
-\varepsilon_{33} I_{v,333} = \varepsilon_{33} I_{\phi,333}^{(1)} + \varepsilon_{11} A_r \phi^{(1)} = -q I_{n,333}^{(1)}.
\]

The substitution of equation (6) into equation (2)_4 gives

\[
-n_0 \mu_3^n I_{\phi,333}^{(1)} = D_{33} n_{\phi,333}^{(1)} + n_0 \mu_3^n A_r \phi^{(1)} - D_{11} n_{\phi,333}^{(1)} = I_{n,333}^{(1)}.
\]

Equations (13)–(15) are the three equations needed for \( v, \phi^{(1)} \), and \( n^{(1)} \).
3. Buckling of a simply-supported fiber

For the static buckling analysis in this paper, all the inertia terms in the above equations vanish, and equation (13) needs to be modified by adding a term due to a compressive axial force \( P \) according to [45] in the following manner:

\[
-\varepsilon_{33} I v_{3333} + \varepsilon_{33} I \phi_{333}^{(1)} - P v_{33} = 0. \tag{16}
\]

\( P \) is applied while the two ends of the fiber are electrically shorted so that \( P \) produces an axial stress only without any axial electric field or carrier redistribution. Then the two ends of the fiber are opened during the buckling process. In this section we consider a fiber simply-supported at \( x_3 = 0 \) and \( L \). We have the following boundary conditions for the fields associated with the bending deformation during buckling:

\[
\begin{align*}
v &= 0, \\
M_i &= -\varepsilon_{33} I v_{33} + \varepsilon_{33} I \phi_{3}^{(1)} = 0, \\
D_i^{(1)} &= -\varepsilon_{33} I v_{33} - \varepsilon_{33} I \phi_{3}^{(1)} = 0, \\
J_n^{(1)} &= -q n_0 \mu_{33}^p I \phi_{3}^{(1)} + q D_{33}^n I \phi_{n}^{(1)} = 0. \tag{17}
\end{align*}
\]

We need to solve equations (14)–(16) under equation (17). Consider the following fields as a trial solution:

\[
\begin{align*}
v &= A_1 \sin \frac{m \pi}{L} x_3, \\
\phi^{(1)} &= B \cos \frac{m \pi}{L} x_3, \\
\eta^{(1)} &= C \cos \frac{m \pi}{L} x_3, \\
m &= 1, 2, 3 \ldots,
\end{align*}
\tag{18}
\]

where \( A, B \) and \( C \) are undetermined constants. It can be verified that equation (18) satisfies equation (17). Substituting equation (18) into the static forms of equations (14)–(16), we obtain three homogeneous linear algebraic equations for \( A, B, \) and \( C \). For nontrivial solutions, the determinant of the coefficient matrix of the three linear equations has to vanish, which leads to an equation for \( P \) whose roots determine the critical buckling loads denoted by \( P_{cr} \). The corresponding nontrivial solutions of \( A, B, \) and \( C \) determine the corresponding buckling modes for the deflection curve, electric potential, and carrier concentration perturbation. The buckling load \( P_{cr} \) is found to be

\[
P_{cr} = P_{cr}^0 \left[ 1 + \frac{\tilde{k}_{33}^2}{\varepsilon_{33} I \left( \frac{m \pi}{L} \right)^2} \right], \tag{19}
\]

where we have denoted

\[
P_{cr}^0 = \varepsilon_{33} I \left( \frac{m \pi}{L} \right)^2, \quad \tilde{k}_{33}^2 = \frac{m \pi}{\varepsilon_{33} I}.
\tag{20}
\]

\( P_{cr}^0 \) is the buckling load of the corresponding elastic dielectric fiber when electromechanical couplings are neglected. \( \tilde{k}_{33}^2 \) is the axial electromechanical coupling coefficient describing the strength of the coupling. Its role in equation (19) represents the well-known piezoelectric stiffening effect which tends to increase the buckling load. The effect of semiconduction represented by the \( n_0 \) term in the denominator of equation (19) tends to reduce the piezoelectric stiffening because of the screening effect of the electrons on the piezoelectrically produced electric field, and hence lower the buckling load. When \( n_0 \) is set to zero in equation (19), we have the following critical buckling load \( P_{cr}^0 \) of the corresponding piezoelectric dielectric fiber:

\[
P_{cr}^0 = P_{cr}^0 \left[ 1 + \frac{\tilde{k}_{33}^2}{\varepsilon_{33} I \left( \frac{m \pi}{L} \right)^2} \right]. \tag{21}
\]

When further neglecting the electromechanical coupling effect or piezoelectricity, namely, we set \( \tilde{k}_{33} \) and \( n_0 \) to be zero in equation (19). Thus, the critical buckling load for pure elastic rods is obtained as

\[
P_{cr}^0 = P_{cr} = \varepsilon_{33} I \left( \frac{m \pi}{L} \right)^2,
\]

which is identical with that in [46]. This indicates the present analytical model is correct.
4. Numerical results and discussion

As a numerical example, we consider a ZnO fiber of radius \( a = 25 \text{ nm} \), length \( L = 600 \text{ nm} \), and initial carrier concentration \( n_0 = 10^{23} / \text{m}^3 \). \( L \) and \( n_0 \) will be varied separately below. Figure 2(a) shows the effect of \( L \) on the piezoelectric semiconductor buckling load \( P_{cr} \), the piezoelectric dielectric buckling load \( P_{cr}^p \), and the elastic dielectric buckling load \( P_{cr}^e \). The buckling loads decay rapidly as \( L \) increases. The three buckling loads are very close, suggesting that the piezoelectric coupling and the related stiffening effect are not strong in ZnO. A magnified local view does show that \( P_{cr}^p \) is higher than \( P_{cr}^e \) as expected due to the piezoelectric stiffening effect, but only by a small amount. The screening effect of the electrons weakens the piezoelectric stiffening and lowers \( P_{cr}^p \) a little to \( P_{cr} \) which is still above \( P_{cr}^e \) as expected. In figure 2(b) which is for a piezoelectric semiconductor fiber only, as \( n_0 \) increases, there are more electrons, the screening effect of the electrons becomes stronger, the piezoelectric stiffening becomes less, and the buckling load decreases as expected.

Figure 3 shows the first three buckling modes corresponding to \( m = 1, 2, \) and 3. They are normalized according to

\[
\tilde{x}_3 = \frac{x_3}{L}, \quad v = \sin m \pi \tilde{x}_3, \\
\tilde{\theta}^{(1)} = \cos m \pi \tilde{x}_3, \quad \tilde{\phi}^{(1)} = \cos m \pi \tilde{x}_3.
\]

These modes are very simple and are as expected for a simply supported fiber. It can be seen from equation (22) that \( \tilde{\phi}^{(1)} \) is the same as \( \tilde{\theta}^{(1)} \). Therefore the mode of \( \tilde{\phi}^{(1)} \) is not shown.
For a piezoelectric semiconductor fiber, we are particularly interested in the carrier concentration perturbation $\Delta n$, which is normalized according to

$$\bar{x}_2 = x_2/a, \quad \bar{n} = x_2 \cos m\pi x_3,$$

and is shown in figure 4 for $m = 1, 2, 3$. The figure shows that the electrons move toward the top and bottom (the lateral surface) of the fiber during buckling, and that $\Delta n$ alternates its sign across nodal points (zeros) when $m=2$ and $3$. We note that the average of $\Delta n$ over a cross section is zero. Therefore, this buckling induced $\Delta n$ does not contribute directly to the axial flow of electrons in a device operating with the extensional deformation of the fiber [15], but it does produce a lateral electric field that acts on the electrons. The electrons move towards the two lateral sides of the fiber under the driving of piezoelectric field. Interestingly, there are more local converging regions of electrons along the bending direction of the fiber when increasing $m$. This buckling induced phenomenon may be used to make multichannel electronic devices, which is very similar to the vibration-induced one in [47]. The distribution of the normalized $\varphi$ looks the same as $\Delta n$, which is not presented here.

5. Fibers with other end supports

Equations equations (19)–(21) are for a fiber simply supported at both ends. For fibers with other end supports, the critical buckling loads can be determined using the concept of the effective length of a fiber according to the mechanics of materials [46] as described below.

For elastic fibers in the most important buckling mode corresponding to $m = 1$, it is known that the expression for the buckling load in equation (20) for a simply supported fiber can be used for fibers with other end supports when the length $L$ in equation (20) is replaced by the effective length $KL$ [46], i.e.,

$$p_{cr}^* = \frac{\pi^2 E_2 I}{(KL)^2},$$

where the values of $K$ for various combinations of end supports are given in table 1. In the table, a fiber with two simply supported ends corresponds to the reference case listed as b-b with $K = 1$. For other cases, consider a fiber with two fixed ends or the case listed as a-a as an example. The table shows a value of $K = 0.5$ which, when substituted into equation (24), quadruples the buckling load of a simply supported fiber. This is reasonable because it takes a larger axial load to buckle a fiber with two fixed ends. For elastic dielectric fibers, the effective length yields the exact buckling loads for different end conditions. For the piezoelectric semiconductor fibers, we

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Figure 4. Buckling modes of normalized $\Delta n$. (a) $m = 1$. (b) $m = 2$. (c) $m = 3$. 

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Mater. Res. Express 6 (2019) 125919 C Liang et al
are considering, the effective length may be approximate but it should be very accurate in view of the weak piezoelectric stiffening effect shown in figure 2.

In [48], the buckling experiment of the fixed-fixed ZnO fiber with length of 2000 nm and radius of 50 nm was conducted. In this case, \( K = 0.5 \), we use the developed model to calculate its critical buckling load. Because the concentration of electrons of ZnO is not given in [48], we compute the case of \( n_0 \) from \( 10^{20} \) to \( 10^{25} \) m\(^{-3} \) and plot it in figure 5. It can be seen that the theoretical critical buckling load of the fixed-fixed piezoelectric semiconductor fiber lies between \( P_{cr} = 6.981 \mu N \) and \( P_{cr} = 6.984 \mu N \). It agrees well with the experimental result of \( 5.68 \mu N \) in [48]. In addition, as the ZnO fiber was grown on an elastic substrate in [48], while the ideal fixed-fixed boundary condition is used in the theoretical calculation. Hence, it is reasonable that the theoretical critical buckling load has a little larger than that in the experimental test.

6. Fiber arrays

Piezoelectric semiconductor fiber-based devices are often fabricated as fiber arrays between two films (see figure 6), which usually operate under a pressure [10]. In this section we use the buckling load for a single fiber in equation (19) to determine a buckling pressure of an array structure.

Specifically, consider the ZnO fiber array structure studied in [49]. The fibers have a tip diameter \( 2a = 300 \text{ nm} \) and \( L = 4 \mu \text{m} \). Since the effect of piezoelectric stiffening on the buckling load of ZnO fibers is small, we use \( P_v \cong P_{cr}^{a} \) as an approximation. According to the experimental model employed in [49], the fibers are treated as with both ends fixed (\( K = 0.5 \)). For a single fiber, calculation shows that

\[
P_v \cong P_{cr}^{a} = \frac{\pi^2 \varepsilon_0 I}{(KL)^2} = 1.4137 \times 10^{-4} \text{ N. (25)}
\]

In [49], the film area is \( S = 4 \text{ mm}^2 \), the total number of nanowires are about \( N_f = 75000 \). The fiber areal density is \( 1.875 \times 10^6 \text{ cm}^{-2} \). Hence, the total critical pressure on the film can be calculated from the theoretical

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Table 1. \( K \)-factors for fibers with different combinations of end conditions.

| End conditions | Theoretical \( K \)-value |
|----------------|--------------------------|
| a–a            | 0.5                      |
| a–b            | 0.7                      |
| a–c/b–b        | 1.0                      |
| a–d/b–c        | 2.0                      |

End condition code:
- a. Rotation fixed and translation fixed
- b. Rotation free and translation fixed
- c. Rotation fixed and translation free
- d. Rotation free and translation free

Figure 5. Theoretical critical buckling loads of the fixed-fixed ZnO fiber with \( L = 2000 \text{ nm} \) and \( R = 50 \text{ nm} \) for different \( n_0 \).
critical load of equation (5) of a single fiber. It is
\[
\sigma_c = \frac{N_s}{S} \cong 2.65 \text{ MPa.} \tag{26}
\]

In [49], pressures of 1.25, 2.5, 3.75 and 6.25 MPa were actually applied experimentally, suggesting the possible involvement of buckling.

7. Conclusions

We present a static buckling model for piezoelectric semiconductor fibers by taking the coupling of deformation, polarization, and carriers into consideration. It is an extension of classical elastic and piezoelectric buckling models. Exact buckling loads and modes for a simply supported piezoelectric semiconductor fiber are obtained from a one-dimensional model. For a ZnO fiber, the buckling loads are only slightly higher than the corresponding elastic dielectric buckling load because the piezoelectric coupling and stiffening effect are small and are further weakened by the screening effect of the electrons. During buckling, the electrons move toward the lateral surface of the fiber, alternating across the nodal points in higher buckling modes. The buckling-induced \( \Delta n \) does not contribute directly to the average flow of electrons over a cross section, but it produces a lateral electric field that acts on the electrons. The buckling loads of the simply supported fiber are extended to fibers with other end supports using the concept of effective length from the mechanics of materials approximately. The buckling pressure of a fiber array between two films is also determined. Calculations show that buckling may be present in some fiber array devices in the literature. In addition, it is desirable to verify experimentally the developed static buckling model of a piezoelectric semiconductor fiber.

It should be also noted the size-dependent behaviors of structures are not our concern and are thus not considered in this paper. However, the size effects such as surface effect, flexoelectricity, strain gradient and nonlocal effect play a significant role in macroscopic mechanical behavior of structures at nanoscale. Some researchers have presented nonlocal model for elastic beams and studied their size-dependent properties [50–53]. For piezoelectric semiconductor structures at nano-scale, it is very necessary to develop a multi-field coupling model which can predict the size-dependent behaviors in the future.

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