Effects of an attached functionally graded layer on the electromechanical behaviors of piezoelectric semiconductor fibers

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(Received Mar. 15, 2022 / Revised Jul. 8, 2022)

Abstract In this paper, we propose a specific two-layer model consisting of a functionally graded (FG) layer and a piezoelectric semiconductor (PS) layer. Based on the macroscopic theory of PS materials, the effects brought about by the attached FG layer on the piezotronic behaviors of homogeneous n-type PS fibers and PN junctions are investigated. The semi-analytical solutions of the electromechanical fields are obtained by expanding the displacement and carrier concentration variation into power series. Results show that the antisymmetry of the potential and electron concentration distributions in homogeneous n-type PS fibers is destroyed due to the material inhomogeneity of the attached FG layer. In addition, by creating jump discontinuities in the material properties of the FG layer, potential barriers/wells can be produced in the middle of the fiber. Similarly, the potential barrier configuration near the interface of a homogeneous PS PN junction can also be manipulated in this way, which offers a new choice for the design of...
PN junction based devices.

Key words  piezoelectric semiconductor (PS), functionally graded (FG) material, composite structure, PN junction

Chinese Library Classification  O472+.91
2010 Mathematics Subject Classification  82D37

1 Introduction

The third-generation semiconductor materials represented by ZnO and GaN are drawing increasing attention due to their excellent features, such as higher thermal conductivity, wider band gap, and bigger electron saturation rate\[1\]. Most third-generation semiconductors also possess piezoelectricity. They are commonly known as piezoelectric semiconductors (PSs)\[2–3\]. When a strain is applied on a PS medium, the electric field induced by the piezoelectric effect will drive the redistribution of free carriers, thus enabling mechanical manipulation of semiconductor behaviors. This unique interaction among deformation, polarization, and mobile charges can be used to develop new electronic devices such as nanogenerators\[4\], piezotronic field-effect transistors\[5–6\], and physical and chemical sensors\[7–8\], as well as piezotronic logic nanodevices\[9\]. To reveal the physical mechanism of PS devices from an applied science perspective, a macroscopic theory consisting of the conventional piezoelectric equations and the conservation of charge for electrons and holes was proposed and has been used to study various problems, including wave propagation\[10\], cracks\[11\], extension and bending of fibers\[12–13\], and potential barrier configuration of PN junctions\[14\]. Very recently, the effects of flexoelectricity\[15\], temperature\[16\], and magnetic field\[17\] were also taken into consideration. These studies provide the theoretical basis for the design and fabrication of PS devices.

One-dimensional fiber in extension mode is widely used in PS devices\[18–19\]. Its electromechanical properties have been numerically\[20\] and theoretically\[12\] studied. Different from the linearly distributed electric potential in a conventional piezoelectric dielectric fiber, the potential in the extensional PS fiber varies very rapidly near the two ends and is almost antisymmetric about the midpoint. However, it was demonstrated by Araneo et al.\[21\] that this antisymmetry may not be optimal for designing devices with high performance. They further suggested that adopting a conical contour of the fiber could break this antisymmetry and thus obtain a higher on-off ratio, which can actually be attributed to the non-uniform strain produced in the inhomogeneous fiber. In addition, another study showed that the non-uniform strain applied to a PS PN junction results in a large increase in the sensitivity\[22\]. Therefore, it is desirable to develop more approaches for creating non-uniform strain in PS fibers, which is just the original intention of this contribution.

Functionally graded (FG) materials are multiphase composites whose phase volume fractions vary with space in a predetermined profile\[23–24\]. Appropriate phase ratios endow FG materials with superior properties compared to conventional composites. Therefore, they have been extensively used in automotive applications\[25\], aerospace vehicles\[26\], military equipment\[27\], and biomedical components\[28\]. Recently, some researchers have attempted to apply FG materials to the field of PSs. Chu et al.\[29\] theoretically studied the electromechanical fields in FG semiconductor nanobeams. Using the finite element method, Lu et al.\[30\] and Sladek et al.\[31\] investigated the electrical behavior of FG PS beams under different loads. Sladek et al.\[32\] presented a dynamic analysis of an anti-plane crack in FG PSs. In spite of these studies, research on FG PS materials is still very scarce.

Given the fact that FG materials are inhomogeneous composites with properties varying in space, the strain produced in an extensional/compressional PS fiber must be non-uniform when an FG layer is attached to it. Therefore, a two-layer model consisting of an FG layer and a PS layer is proposed in this paper. A series of theoretical analyses are conducted to investigate
the electromechanical behaviors of this composite structure. In Section 2, the linearized one-
dimensional coupled equations for the proposed two-layer model are established, followed by the
semi-analytical solutions of the electromechanical fields and the corresponding iterative process.
Then, the boundary conditions of the extensional composite fiber with a PN junction are
displayed in Section 3. The effects of the FG layer on the piezotronic properties of homogeneous
n-type PS fibers and PN junctions are discussed as numerical examples in Section 4. Finally,
some conclusions are summarized in Section 5.

2 One-dimensional theoretical model and semi-analytical solutions

Consider the thin composite fiber consisting of a bottom PS layer and a top FG layer shown
in Fig. 1. The bottom PS layer possesses both piezoelectricity and semiconducting property and
is assumed to be uniformly doped with donors N_D^+ and acceptors N_A^- . Its poling direction is
parallel to the x_3-axis. The top FG layer possesses only piezoelectricity and no semiconducting
property. Its material coefficients, including the elastic coefficient, piezoelectric coefficient, and
dielectric coefficient, vary along the x_3-axis. A pair of equal and opposite axial forces F are
applied at the two ends of the composite fiber. When F = 0, the fiber is at the reference state,
and the electron and hole concentrations are respectively n_0 = N_D^+ and p_0 = N_A^- . When F ≠ 0,
variations Δp and Δn of hole and electron concentrations occur due to the interaction between
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where \( \mu_{33}^p(\mu_{33}^g) \) and \( D_{33}^p(D_{33}^g) \) represent the carrier mobility and carrier diffusion constants, respectively. The axial strain \( S_3 \) and electric field \( E_3 \) are defined respectively as

\[
S_3 = u_{3,3}, \quad E_3 = -\varphi_{,3}. \tag{6}
\]

The one-dimensional effective elastic coefficient \( \hat{c}_{33} \), piezoelectric coefficient \( \hat{e}_{33} \), and dielectric coefficient \( \hat{a}_{33} \) in Eq. (4) are

\[
\begin{align*}
\hat{c}_{33} &= c_{33}^{(1)} + c_{33}^{(2)} = c_{33}^{(1)}A^{(1)} + c_{33}^{(2)}A^{(2)}, \\
\hat{e}_{33} &= e_{33}^{(1)} + e_{33}^{(2)} = e_{33}^{(1)}A^{(1)} + e_{33}^{(2)}A^{(2)}, \\
\hat{a}_{33} &= a_{33}^{(1)} + a_{33}^{(2)} = a_{33}^{(1)}A^{(1)} + a_{33}^{(2)}A^{(2)}.
\end{align*}
\tag{7}
\]

The usual stress relaxation approximation for thin fibers requires\([12,34]\)

\[
e_{33}^{(1)} = 1/s_{33}^{(1)}, \quad e_{33}^{(1)} = a_{33}^{(1)/s_{33}^{(1)}}, \quad a_{33}^{(1)} = a_{33}^{(1)} - (d_{33}^{(1)}/s_{33}^{(1)}),
\]

where \( s_{33}^{(1)} \) is the elastic compliance, and \( d_{33}^{(1)} \) is the piezoelectric constant, and \( a_{33}^{(1)} \) is the dielectric constant. Due to the the existence of the top FG layer, the total effective material coefficients \( \hat{c}_{33}, \hat{e}_{33}, \) and \( \hat{a}_{33} \) of the composite fiber are dependent on the coordinate \( x_3 \). Regardless of how these effective material coefficients vary along the \( x_3 \)-axis, they can be theoretically expanded into power series\([35]\),

\[
\begin{align*}
\hat{c}_{33} &= \left[C_0 + C_1 \left(\frac{x_3}{L}\right) + C_2 \left(\frac{x_3}{L}\right)^2 + \cdots\right] = \sum_{f=0}^{M_f} C_f \left(\frac{x_3}{L}\right)^f, \\
\hat{e}_{33} &= \left[E_0 + E_1 \left(\frac{x_3}{L}\right) + E_2 \left(\frac{x_3}{L}\right)^2 + \cdots\right] = \sum_{g=0}^{M_g} E_g \left(\frac{x_3}{L}\right)^g, \\
\hat{a}_{33} &= \left[A_0 + A_1 \left(\frac{x_3}{L}\right) + A_2 \left(\frac{x_3}{L}\right)^2 + \cdots\right] = \sum_{k=0}^{M_k} A_k \left(\frac{x_3}{L}\right)^k,
\end{align*}
\]

where \( M_f, M_g, \) and \( M_k \) are the series truncation parameters, and \( C_f, E_g, \) and \( A_k \) the graded coefficients. Note that the effective material coefficients \( \hat{c}_{33}, \hat{e}_{33}, \) and \( \hat{a}_{33} \) of the PS layer have already been included in the constant terms of these series. For the static problems to be considered in this paper, the isolated boundary condition requires \( J_3^p = J_3^g = 0 \) in Eq. (5), which leads to

\[
\Delta n_{,3} = n_0 \frac{\mu_{33}^p}{D_{33}^p} \varphi_{,3}, \quad \Delta p_{,3} = -p_0 \frac{\mu_{33}^g}{D_{33}^g} \varphi_{,3}. \tag{10}
\]

Subtracting these two equations from each other, we get

\[
\varphi_{,3} = \frac{1}{n_0 \frac{\mu_{33}^p}{D_{33}^p} + p_0 \frac{\mu_{33}^g}{D_{33}^g}} (\Delta n - \Delta p)_{,3} = M(\Delta n - \Delta p)_{,3}. \tag{11}
\]

The Einstein relation is

\[
\mu_{33}^n \frac{D_{33}^p}{D_{33}^g} = \mu_{33}^p \frac{D_{33}^g}{D_{33}^n} = \frac{q}{k_B T}, \tag{12}
\]

where \( k_B \) is the Boltzmann constant, and \( T \) is the absolute temperature. With the use of Eqs. (4), (6), and (11), we can rewrite Eq. (2) as

\[
\begin{align*}
\hat{c}_{33,3} u_{3,3} + \hat{c}_{33} u_{3,3} + \hat{e}_{33} M(\Delta n - \Delta p)_{,3} + \hat{a}_{33} M(\Delta n - \Delta p)_{,3} &= 0, \\
\hat{c}_{33,3} u_{3,3} + \hat{c}_{33} u_{3,3} - \hat{a}_{33} M(\Delta n - \Delta p)_{,3} - \hat{a}_{33} M(\Delta n - \Delta p)_{,3} &= q A^{(1)}(\Delta p - \Delta n).
\end{align*}
\tag{13}
\]

It is difficult to obtain the exact analytical solution to this system of partial differential equations due to the variable coefficients. Herein, we will use a power series expansion method.
to get the semi-analytical results. Expanding the displacement \( u_3 \) and carrier concentration variation \( \Delta n - \Delta p \) into power series yields

\[
\left\{
\begin{array}{l}
u = \left( U_0 + U_1 \left( \frac{x_3}{L} \right) + U_2 \left( \frac{x_3}{L} \right)^2 + \cdots \right) = \sum_{s=0}^{M_s} U_s \left( \frac{x_3}{L} \right)^s, \\
\Delta n - \Delta p = \left( N_0 + N_1 \left( \frac{x_3}{L} \right) + N_2 \left( \frac{x_3}{L} \right)^2 + \cdots \right) = \sum_{s=0}^{M_s} N_s \left( \frac{x_3}{L} \right)^s
\end{array}
\right. \tag{14}
\]

with the series truncation parameter \( M_s \). Coefficients \( U_s \) and \( N_s \) will be determined later with the use of specific boundary conditions. Substituting Eqs. (9) and (14) into Eq. (13) yields

\[
\left\{
\begin{array}{l}
\frac{1}{L^2} \sum_{f=1}^{M_f} f C_f \left( \frac{x_3}{L} \right) f-1 \sum_{s=1}^{M_s} s U_s \left( \frac{x_3}{L} \right)^{s-1} + \frac{1}{L^2} \sum_{f=0}^{M_f} C_f \left( \frac{x_3}{L} \right) \sum_{s=2}^{M_s} s(s-1) U_s \left( \frac{x_3}{L} \right)^{s-2} \\
+ \frac{1}{L^2} \sum_{g=1}^{M_g} g E_g \left( \frac{x_3}{L} \right) g-1 \sum_{s=1}^{M_s} s N_s \left( \frac{x_3}{L} \right)^{s-1} + \frac{1}{L^2} \sum_{g=0}^{M_g} E_g \left( \frac{x_3}{L} \right) \sum_{s=2}^{M_s} s(s-1) N_s \left( \frac{x_3}{L} \right)^{s-2} \\
= 0,
\end{array}
\right. \tag{15}
\]

In order for Eq. (15) to hold for an arbitrary \( x_3 \), the coefficients of \( (x_3/L)^s \) should be zero.

This gives

\[
\left\{
\begin{array}{l}
\frac{1}{L^2} \sum_{f=0}^{s} (f+1) C_{f+1} (s-f+1) U_{s-f+1} + \frac{1}{L^2} \sum_{f=0}^{s} C_f (s-f+2) (s-f+1) U_{s-f+2} \\
+ M \sum_{g=0}^{s} (g+1) E_{g+1} (s-g+1) N_{s-g+1} + M \sum_{g=0}^{s} E_g (s-g+2) (s-g+1) N_{s-g+2} = 0,
\end{array}
\right. \tag{16}
\]

We can obtain the recursive relationships for \( U_s \) and \( N_s \) from Eq. (16), i.e.,

\[
N_{s+2} = \left\{
\begin{array}{l}
\frac{1}{L^2} \sum_{g=0}^{s} (g+1) E_{g+1} (s-g+1) U_{s-g+1} + \frac{1}{L^2} \sum_{g=1}^{s} E_g (s-g+2) (s-g+1) U_{s-g+2} \\
- \frac{E_0}{C_0 L^2} \sum_{f=0}^{s} (f+1) C_{f+1} (s-f+1) U_{s-f+1} - \frac{E_0}{C_0 L^2} \sum_{f=1}^{s} C_f (s-f+2) (s-f+1) U_{s-f+2}
\end{array}
\right. \]
3 Analysis of electromechanical fields in the composite fiber with a PN junction

Consider the composite fiber shown in Fig. 2. The top layer is the FG layer, and the bottom layer is the PS layer. The right half of the PS layer is the electron-dominated n-type region, and the left is the hole-dominated p-type region. The material of these two parts may be the same (homogeneous junction) or different (heterogeneous junction), both of which will be discussed in the numerical example section.

Equation (17) indicates that there are four unknown coefficients $N_0$, $N_1$, $U_0$, and $U_1$ to be determined. Other $N_s$ and $U_s$ for $s > 1$ can be calculated using these two recursive relationships. Then, the distributions of $u_3$ and $\Delta n - \Delta p$ can be calculated using Eq. (14). Equation (10) gives the expression for $\Delta n$ as

$$\Delta n = n_0 \frac{\mu_{33}^n}{D_{33}} M (\Delta n - \Delta p) + P_1 = n_0 \frac{\mu_{33}^n}{D_{33}} M \sum_{s=0}^{M_s} N_s \left( \frac{x_3}{L} \right)^s + P_1, \quad (18)$$

in which $P_1$ is an undetermined constant. Further, $\Delta p$ can be calculated by

$$\Delta p = \Delta n - (\Delta n - \Delta p) = \left( n_0 \frac{\mu_{33}^n}{D_{33}} M - 1 \right) \sum_{s=0}^{M_s} N_s \left( \frac{x_3}{L} \right)^s + P_1. \quad (19)$$

For this composite fiber containing a PN junction, the $x_3 \leq 0$ and $x_3 > 0$ regions need to be treated separately. Note that the field equations and iterative relationships derived in Section 2 hold for both regions. Therefore, ten unknown constants, five for $x_3 \leq 0$ and five for $x_3 > 0$, need to be determined. The boundary conditions for the considered composite structure are

$$\hat{T}_3(L) = F, \quad u(-L) = 0, \quad \hat{D}_3(L) = 0, \quad \hat{D}_3(-L) = 0. \quad (20)$$
The continuity conditions are
\[
\begin{align*}
\dot{T}_3(0^-) &= \dot{T}_3(0^+), & u(0^-) &= u(0^+), & \dot{D}_3(0^-) &= \dot{D}_3(0^+), \\
n(0^-) &= n(0^+), & p(0^-) &= p(0^+).
\end{align*}
\]
In addition, the following global charge neutrality condition needs to be satisfied:
\[
\int_{-L}^{L} (\Delta p - \Delta n) dx_3 = 0.
\]
With the use of Eqs. (20), (21), and (22), the semi-analytical solutions for the displacement and carrier concentration variations can be obtained. Then, the distribution of the electric potential \( \varphi \) can be obtained by integrating Eq. (11). The polarization is calculated from
\[
P_3 = \frac{\dot{D}_3}{A^{(1)} + A^{(2)}} - \varepsilon_0 E_3,
\]
where \( \varepsilon_0 \) is the vacuum permittivity. Now, all the physical fields in the composite fiber with a PN junction can be solved in a computer.

4 Numerical examples and discussion

In numerical examples, the material of the bottom layer (both the p-type and n-type regions) is assumed to be ZnO, whose material constants are from Ref. [12]. For homogeneous junctions, the poling directions of the left and right halves are all along the positive \( x_3 \)-axis. While for heterogeneous junctions, we simply reverse the poling directions of the right halves. In this case, the relevant piezoelectric constants change their signs. The cross-sectional areas of the two layers are \( A^{(1)} = A^{(2)} = 2.598 \times 10^{-14} \text{ m}^2 \). The initial concentrations of electrons and holes are \( n_0^l = 7 \times 10^{20} \text{ m}^{-3} \), \( p_0^l = 1 \times 10^{21} \text{ m}^{-3} \), \( n_0^r = 1 \times 10^{21} \text{ m}^{-3} \), and \( p_0^r = 7 \times 10^{20} \text{ m}^{-3} \) unless otherwise specified. Note that in this paper, we use superscript ‘l’ for the physical quantities of the left part \( (x_3 < 0) \) and superscript ‘r’ for the right \( (x_3 > 0) \). We retain only two terms in the series of each effective material coefficient in Eq. (9), which is sufficient to reveal the effects brought about by the FG layer on the electromechanical properties of the PS fiber. Hence, the effective material coefficient for the left and right halves of the composite fiber can be rewritten as
\[
\begin{align*}
\tilde{c}_{33}^l &= \lambda_{c33}^l c_{33}^{(1)l} + \beta_{c33}^l c_{33}^{(1)l} x_3 L, & \tilde{c}_{33}^r &= \lambda_{c33}^r c_{33}^{(1)r} + \beta_{c33}^r c_{33}^{(1)r} x_3 L, \\
\tilde{c}_{3}^l &= \lambda_{c}^l c_{33}^{(1)l} + \beta_{c}^l c_{33}^{(1)l} x_3 L, & \tilde{c}_{3}^r &= \lambda_{c}^r c_{33}^{(1)r} + \beta_{c}^r c_{33}^{(1)r} x_3 L, \\
\tilde{a}_{33}^l &= \lambda_{a33}^l a_{33}^{(1)l} + \beta_{a33}^l a_{33}^{(1)l} x_3 L, & \tilde{a}_{33}^r &= \lambda_{a33}^r a_{33}^{(1)r} + \beta_{a33}^r a_{33}^{(1)r} x_3 L.
\end{align*}
\]
As mentioned in Section 2, \( c_{33}^{(1)l}, c_{33}^{(1)r}, c_{33}^{(1)l}, c_{33}^{(1)r}, \) \( a_{33}^{(1)l}, \) and \( a_{33}^{(1)r} \) are the effective material constants of the left and right halves of the bottom ZnO layer, respectively. They are used as reference values to describe the material property variations of the composite fiber. Combined with the graded coefficients \( \lambda \) and \( \beta \), the material gradation profiles can be determined.

4.1 Convergence verification

To examine the convergence of the power series expansion method, we calculate the values of coefficients \( N_0^l \) and \( N_0^r \) respectively for a homogeneous junction and a heterogeneous junction. The results for different truncation parameters \( M_4 \) are displayed in Table 1. It shows that the coefficients of the series in Eq. (14) are already stable with about 34 terms kept. To ensure the computational accuracy, we will keep 60 terms in series in the following simulations.

4.2 Numerical validation

The correctness and accuracy of the power series expansion method should be validated. We find that for the composite fiber with a homogeneous junction, if we set \( \lambda_{c}^{1/r} = \lambda_{a}^{1/r} = 1, \beta_{c}^{1/r} = \beta_{a}^{1/r} = 0, n_0^l = n_0^r = 1 \times 10^{21} \text{ m}^{-3} \), and \( p_0^l = p_0^r = 0 \), the effect of the FG layer

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Table 1  Coefficients $N'_0$ and $N''_0$ for different truncations $M_s$ ($\lambda/e = \lambda'/e = 1.5$, and $\beta/e = \beta'/e = 0.5$)

| $M_s$ | $N'_0$ | $N''_0$ | $M_s$ | $N'_0$ | $N''_0$ |
|-------|--------|---------|-------|--------|---------|
| 30    | $3.03680 \times 10^{-20}$ | $-2.96320 \times 10^{-20}$ | 32    | $5.43395 \times 10^{-20}$ | $-5.66054 \times 10^{-19}$ |
| 32    | $3.03678 \times 10^{-20}$ | $-2.96322 \times 10^{-20}$ | 34    | $5.43395 \times 10^{-20}$ | $-5.66055 \times 10^{-19}$ |
| 36    | $3.03678 \times 10^{-20}$ | $-2.96322 \times 10^{-20}$ |       |        |         |

will disappear and the model will degenerate to the case of a homogeneous n-type PS fiber. The analytical solutions of the electromechanical fields in this n-type fiber when $F = 8.5$ nN and $L = 0.6 \mu$m have already been given in Ref. [36]. We compare the electron concentration variations $\Delta n$ obtained respectively from the analytical and semi-analytical solutions in Fig. 3. It can be seen that the results agree well with each other, indicating that the power series expansion method adopted in this paper is valid for the following analyses.

Fig. 3  Electron concentration variations $\Delta n$ obtained from the analytical solution in Ref. [36] and the semi-analytical solution in the present paper (color online)

4.3 Composite fiber with a homogeneous n-type PS layer

For the composite fiber with a homogeneous PN junction, if we set $n'_0 = n''_0 = 1 \times 10^{21}$ m$^{-3}$ and $p'_0 = p''_0 = 0$, its bottom layer will no longer be a PN junction, but a homogeneous n-type fiber, just as the model shown in Fig. 1. Therefore, we can first investigate the effect of the attached FG layer on the electromechanical properties of homogeneous n-type PS fibers. We assume that $\lambda/e = \lambda'/e = 1$ and $\beta/e = \beta'/e = 0$, i.e., only the elastic coefficients of the FG layer vary continuously along the $x_3$-axis, while the piezoelectric and dielectric coefficients are both constants. The electromechanical field distributions are studied for three cases: Case 1, $\lambda/e = 1.5$ and $\beta/e = 0$; Case 2, $\lambda/e = 1.5$ and $\beta/e = 0.25$; Case 3, $\lambda/e = 1.5$ and $\beta/e = 0.5$. These three cases correspond to three different stiffness distributions, which are visualized in Fig. 4(a), where the distributions of the effective elastic coefficient $\tilde{c}_{e3}$ are plotted. It shows that Case 3 has the most non-uniform stiffness distribution, Case 2 the second, and Case 1 the most uniform. Figures 4(b)–4(c) show the distributions of the electric potential $\varphi$, electron concentration variation $\Delta n$, axial strain $S_{33}$, and polarization $P_3$ for these three cases when $F = 8.5$ nN and $L = 0.6 \mu$m. It can be seen from Figs. 4(b) and 4(c) that the potential and electron concentration vary dramatically near the two ends of the fiber, which shows the typical screening effect of mobile charges on the electric potential in PS materials[12,31]. In Case 1, the distributions of $\varphi$ and $\Delta n$ are almost antisymmetric. However, this antisymmetry is broken as the stiffness distribution becomes non-uniform (Case 2 and Case 3). We note that Araneo et al.[21] have previously reported this phenomenon of antisymmetry breaking-off
in conical PS fibers. That is to say, by attaching a FG layer to the homogeneous PS fiber, electromechanical coupling behaviors similar to that of a variable cross-section fiber can be achieved without changing the profile. The strain distributions in Fig. 4(d) are as expected, since the deformation of the softer left half of the composite fiber must be larger than the harder right half. Consequently, a larger polarization $P_3$ is produced on the left due to the piezoelectric coupling, as shown in Fig. 4(e). The polarization charge density on the two end surfaces can be calculated from $P \cdot n$. For Cases 2 and 3, the left surface must have more polarization charges, since the values of $P_3$ there are larger than those on the right surface. They drive more free carriers nearby to redistribute via electrostatic force, leading to the breaking-off of the field antisymmetry.

The results in Fig. 4 are based on the assumption that the material coefficients of the FG layer vary continuously along the fiber (see Fig. 4(a)). Next, another situation of material properties having jump discontinuities will be investigated. Similarly, the effective piezoelectric and dielectric coefficients are set as constants with $\lambda_3^{1/r} = \lambda_3^a = 1$ and $\beta_3^{1/r} = \beta_3^a = 0$. Three different cases of stiffness distribution will be considered. They are: Case 4, $\lambda_3^c = 1.5, \lambda_3^l = 1$, and $\beta_3^{1/r} = 0.5$; Case 5, $\lambda_3^c = 1.5, \lambda_3^l = 1.5$, and $\beta_3^{1/r} = 0.5$; Case 6, $\lambda_3^c = 2, \lambda_3^l = 1.5$, and $\beta_3^{1/r} = 0.5$. The corresponding distributions of the effective elastic coefficient $c_{33}$ are shown in Fig. 5(a). We see that the stiffness in Cases 4 and 6 is discontinuous at $x_3 = 0$ while that in Case 5 is completely continuous. The distributions of electric potential $\varphi$, electron concentration variation $\Delta n$, axial strain $S_3$, and polarization $P_3$ when $F = 8.5\, \text{nN}$ and $L = 0.6\, \mu\text{m}$ are plotted in Figs. 5(b)–5(e). We can see in Figs. 5(b) and 5(c) that the antisymmetry breaking-off phenomenon still exists. In addition, electrons are driven away or toward the stiffness discontinuities, resulting in the appearance of a potential well or barrier. This is because the discontinuous strain $S_3$ induces the jump of polarization $P_3$ at $x_3 = 0$, which produces effective polarization charges with a density of $\sigma^P = P_3(0^-) - P_3(0^+)$ there. The sign of $\sigma^P$ depends on the difference in stiffness between the two sides of the discontinuity. Therefore, the electric behaviors in the middle of a PS fiber can be manipulated by reasonably creating discontinuities in the material coefficients of the attached FG layer.

![Fig. 4](image-url)
4.4 Composite fiber with a PN junction

We now pay attention to the effects of the FG layer on the potential barrier configuration of a PS PN junction. The graded coefficients of the FG layer are firstly assumed to be $\lambda_{33}^{l/r} = \lambda_{33}^{l/r} = 1$, $\beta_{33}^{l/r} = 0$, $\alpha_{33}^{l/r} = 1.5$, and $\beta_{33}^{l/r} = 0.3$, which means that the effective piezoelectric coefficient $\tilde{e}_{33}$ and dielectric coefficient $\tilde{\varepsilon}_{33}$ are both constants, while the elastic coefficient $\tilde{\lambda}_{33}$ varies linearly along the fiber with no jump discontinuities. The length of the two halves is $L = 1.8\,\mu$m. The electric potential distributions respectively in homogeneous and heterogeneous junctions for different values of applied force $F$ are plotted in Figs. 6(a) and 6(b). In order to clearly show the small variations of the potential barrier configuration, only the fields within $|x_3| < 0.6\,\mu$m are plotted. For the homogeneous junction in Fig. 6(a), the increase in $F$ has no influence on the potential barrier near the interface. That is to say, the FG layer with continuously varying material properties cannot be used to manipulate the barrier configuration of homogeneous PS PN junctions. The potential barrier configuration of the heterogeneous junction in Fig. 6(b) varies with the increase in $F$, because the material constants of the ZnO layer itself jump at the interface (reversed $c$-axis). The corresponding distributions of electric field $E_3$ are shown in Figs.6(c) and 6(d). As expected, the curves of $E_3$ for homogeneous junctions overlap each other, while those for heterogeneous junctions vary with $F$. This further proves that the barrier configuration of homogeneous junctions is insensitive to external axial forces.

The discussion in Subsection 4.3 indicates that the jump discontinuities in the material coefficients of the FG layer produce locally distributed polarization charges in the bottom PS layer, which in turn changes the local potential distribution. Inspired by this conclusion, we speculate that the potential barrier configuration of a homogeneous PS PN junction can also be manipulated by attaching an FG layer with discontinuous material coefficients. The graded coefficients of the FG layer are now assumed to be $\lambda_{33}^{l/r} = \lambda_{33}^{l/r} = 1$, $\beta_{33}^{l/r} = \beta_{33}^{l/r} = 0$, $\lambda_{3}^{l} = 4$, $\lambda_{3}^{r} = 1$, and $\beta_{3}^{l/r} = 0.3$. In this case, the effective piezoelectric coefficient $\tilde{e}_{33}$ and dielectric coefficient $\tilde{\varepsilon}_{33}$ are both constants, while the elastic coefficient $\tilde{\lambda}_{33}$ varies linearly along the fiber with a jump discontinuity at the origin. The distributions of potential $\varphi$ and electric field $E_3$ respectively in homogeneous and heterogeneous junctions for different values of $F$ are shown in Fig. 7. Compared to the first column in Fig. 6, the fields near the junction interface in Figs. 7(a) and 7(c) vary with the increasing force $F$, which strongly confirms our previous inference. The field distributions in Figs. 7(b) and 7(d) are similar to those shown in the second column of Fig. 6.
Fig. 6  Distributions of potential $\varphi$ and electric field $E_3$ in PN junctions with material coefficients of the FG layer varying continuously. (a) and (c) for the homogeneous junction; (b) and (d) for the heterogeneous junction (color online)

Fig. 7  Distributions of potential $\varphi$ and electric field $E_3$ in PN junctions with material coefficients of the FG layer varying discontinuously. (a) and (c) for the homogeneous junction; (b) and (d) for the heterogeneous junction (color online)
Therefore, the use of an FG layer with discontinuously varying material coefficients to modulate the potential barrier configuration is effective for both homogeneous and heterogeneous PS PN junctions.

A very recent study suggested that the mechanical loadings applied near the interface lead to an obvious tuning effect on the $I$-$V$ (current-voltage) characteristics of PS PN junctions. Here, we will show that this tuning effect can also be induced by discontinuities in material properties at the interface. Assume that the two ends of the homogeneous junction used for Fig. 7(a) are under an applied voltage $2V$. Then the nonlinear versions of Eqs. (2) and (3) are solved by using the numerical analysis software COMSOL. The $I$-$V$ curves for different values of $F$ are plotted in Fig. 8(a). It shows that the current can be manipulated by the axial force $F$. Further, we keep $F = 3$ nN and change the effective stiffness of the p-type region. The corresponding $I$-$V$ curves plotted in Fig. 8(b) suggest that the current is sensitive to the material property discontinuities at the interface. Therefore, the above-mentioned tuning methodology is feasible.

Fig. 8 Current-voltage relations for different values of (a) applied force $F$ and (b) graded coefficient $\lambda_l$ (color online)

5 Conclusions

In this paper, we theoretically investigate the effects of the attached FG layer on the electromechanical behaviors of one-dimensional PS fibers. The semi-analytical solutions obtained by using the power series expansion method are shown to be capable of producing sufficiently accurate results for both homogeneous n-type fibers and PN junctions. The two cases of continuous and discontinuous variation of the FG layer material properties are discussed separately. Some conclusions can be summarized as follows:

(I) The antisymmetry of the potential and electron concentration distributions in a homogeneous n-type PS fiber is destroyed due to the material inhomogeneity of the attached FG layer.

(II) A potential barrier/well is produced in the middle of the n-type PS fiber as long as there is a jump discontinuity in the material properties of the FG layer.

(III) Even for a homogeneous PS PN junction, the potential barrier configuration near the interface can be manipulated by axial end forces in the presence of an attached FG layer with discontinuously varying material properties.

To summarize, this paper explores a new mechanical manipulation method for PS fibers, which may provide guidance for the development and design of piezotronic devices.

Acknowledgements  Prof. I. E. KUZNETSOVA and Dr. V. KOLESOV thank Russian Ministry of Science and Higher Education (Government task of Kotelnikov IRE of RAS) for partial financial supports. The authors thank to the Start-up Fund by Nanjing University of Aeronautics and Astronautics and the Priority Academic Program Development of Jiangsu Higher Education Institutions (PAPD).
Effects of an attached functionally graded layer on the electromechanical behaviors

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