



Mechanical Manipulation of Electrical Behaviors of Piezoelectric Semiconductor Nanofibers by Time-Dependent Stresses

Haoyu Huang¹ Zhenghua Qian^{1*}  Jiashi Yang²

(¹ State Key Laboratory of Mechanics and Control of Mechanical Structures, College of Aerospace Engineering, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China)

(² Department of Mechanical and Materials Engineering, University of Nebraska-Lincoln, Lincoln, NE 68588-0526, USA)

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ABSTRACT We study electric currents in a piezoelectric semiconductor fiber under a constant voltage and time-dependent axial stresses applied locally. From a nonlinear numerical analysis based on a one-dimensional phenomenological model using the commercial software COMSOL, it is found that pulse electric currents can be produced by periodic or time-harmonic stresses. The pulse currents can be tuned by the amplitude and frequency of the applied stress. The result obtained provides a new approach for the mechanical control of electric currents in piezoelectric semiconductor fibers and has potential applications in piezotronics.

KEY WORDS Piezoelectric semiconductor nanofiber, Tunable pulse electric current, Time-dependent stress, Piezotronics

1. Introduction

Many new piezoelectric semiconductor nanostructures, e.g., ZnO fibers, belts, spirals, tubes and films, have been synthesized in the last one to two decades [1–3]. They have been used to make various electromechanical devices such as energy harvesters, mechanically-gated transistors, acoustic charge transport devices, and physical as well as chemical sensors [4–8]. Piezoelectric semiconductors are also used in quantum wells, dots and wires [9]. The research on piezoelectric semiconductor materials and devices has been growing steadily [10]. It has formed a new research area called piezotronics and piezophotonics [11–14]. In piezotronic devices, the motion of charge carriers is manipulated by mechanical loads through the accompanying electric field due to piezoelectric coupling. Many piezotronic devices are made from ZnO nanofibers with PN or MS junctions [14]. These fibers may be in extensional [15–19] or bending [20–24] deformations, which affect the current–voltage relations (I – V curves) of the junctions. Recently, it has been shown that local extensional/compressive stresses in a piezoelectric semiconductor fiber produce electric potential barriers/wells [25, 26], which affects the I – V curves of the fiber even without the presence of PN or MS junctions. This offers a new means for the mechanical tuning of electrical behaviors of piezoelectric semiconductor fiber devices. The same effect also exists in piezoelectric semiconductor fibers under a local temperature change [27]. In [25, 26], the local stresses

* Corresponding author. E-mail: qianzh@nuaa.edu.cn

are static. They act like a stress-dependent switch in a semiconductor fiber. Under a fixed voltage, current can flow through the fiber when the stress is low, but not so under high stresses. In this paper, we study the effects of time-dependent stresses applied locally in a piezoelectric semiconductor fiber. It is shown that pulse electric currents can be produced and tuned by periodic or time-harmonic stresses.

2. Governing Equations

Consider a piezoelectric semiconductor fiber under a pair of equal and opposite forces F locally at $x = \pm a$ (see Fig. 1). F is time-dependent. The fiber is made from a piezoelectric semiconductor crystal of class (6 mm) such as ZnO. The c -axis of the fiber is along x_3 . The two ends of the fiber are under a constant voltage V . The lateral surface is traction-free and is unelectroded. As an approximation, the electric field in the free space is neglected.

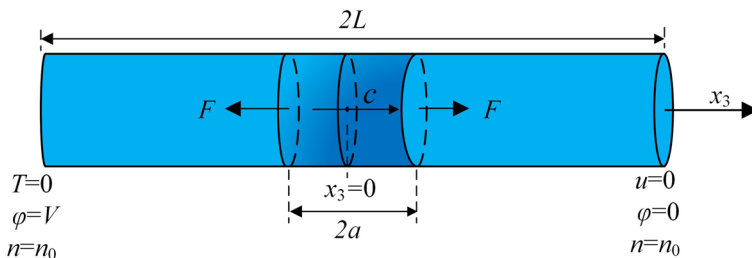


Fig. 1. A piezoelectric semiconductor fiber under local stress

The current–voltage behavior of the fiber can be described by the macroscopic theory of piezoelectric semiconductors, which consists of the classical theory of piezoelectricity [28] and the drift-diffusion theory of semiconductors [29], coupled electrically by the charges in the semiconductor. Specifically, for the extensional motion of a piezoelectric semiconductor fiber, the macroscopic theory can be reduced to a one-dimensional model [15, 26], which is adequate for the purpose of this paper. For the one-dimensional model, the relevant axial fields are denoted by

$$\begin{aligned}
 u_3 &= u(x, t), & \varphi &= \varphi(x, t), \\
 p &= p(x, t), & n &= n(x, t), \\
 S &= S_3(x, t), & E &= E_3(x, t), \\
 T &= T_3(x, t), & D &= D_3(x, t), \\
 J^p &= J_3^p(x, t), & J^n &= J_3^n(x, t)
 \end{aligned}
 \tag{1}$$

where u is the axial displacement, φ the electric potential, p the concentration of holes, n the concentration of electrons, S the strain, T the stress, E the electric field, D the electric displacement, J^p the hole current density, and J^n the electron current density. They are governed by [15, 26]

$$\begin{aligned}
 \frac{\partial T}{\partial x} &= \rho \ddot{u}, \\
 \frac{\partial D}{\partial x} &= q(p - n + N_D^+ - N_A^-), \\
 q \frac{\partial p}{\partial t} &= - \frac{\partial J^p}{\partial x}, \\
 q \frac{\partial n}{\partial t} &= \frac{\partial J^n}{\partial x}
 \end{aligned}
 \tag{2}$$

where ρ is the mass density, q the elementary charge, N_D^+ and N_A^- the concentrations of ionized donors and accepters, respectively. The equations in (2) are Newton’s law, Gauss’s law for electrostatics, and the continuity equations for holes and electrons, respectively. Equations describing material behaviors are [15, 26]

$$T = cS - eE,$$

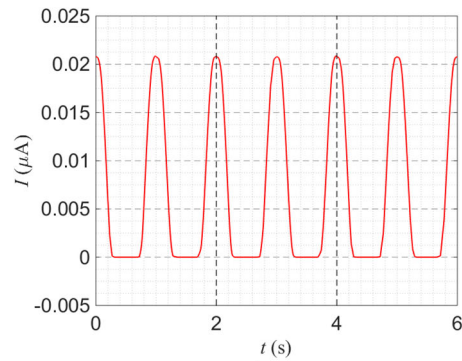
$$D = eS + \varepsilon E \quad (3)$$

$$J^p = qp\mu^p E - qD^p \frac{\partial p}{\partial x},$$

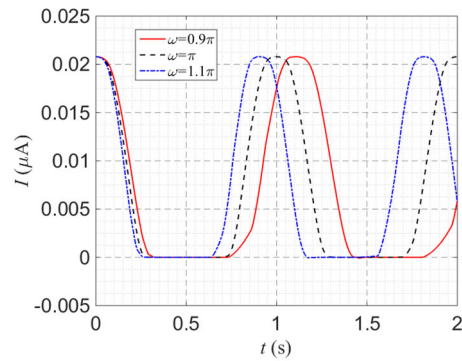
$$J^n = qn\mu^n E + qD^n \frac{\partial n}{\partial x} \quad (4)$$

The mobility μ and the diffusion constants D^p and D^n for holes and electrons in (4) satisfy the following Einstein relation [29]

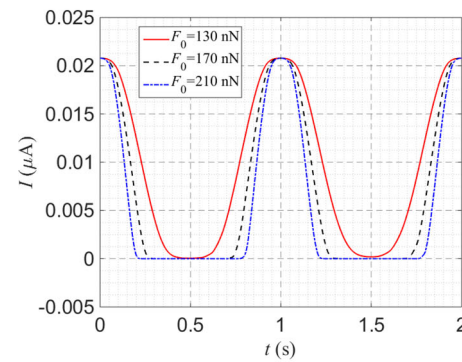
$$\frac{\mu^p}{D^p} = \frac{\mu^n}{D^n} = \frac{q}{k_B \Theta} \quad (5)$$



(a)



(b)



(c)

Fig. 2. Current I in the fiber versus time t under $F = F_0 \cdot \sin(\omega t)$: **a** $F_0 = 170$ nN, $\omega = \pi$; **b** effect of ω when $F_0 = 170$ nN; **c** effect of F_0 when $\omega = \pi$

where k_B is the Boltzmann constant and Θ the absolute temperature. The axial strain–displacement relation and electric field-potential relation are

$$S = \frac{\partial u}{\partial x}, \quad E = -\frac{\partial \varphi}{\partial x} \tag{6}$$

With successive substitutions from (3), (4) and (6), we can write (2) as four equations for u , ϕ , p and n . The boundary conditions are shown in Fig. 1. The initial conditions are

$$\begin{aligned} u &= 0, & \dot{u} &= 0, \\ n &= n_0, & \varphi &= 0 \end{aligned} \tag{7}$$

The above initial-boundary-value problem is solved using COMSOL, a commercial software for numerically solving differential equations.

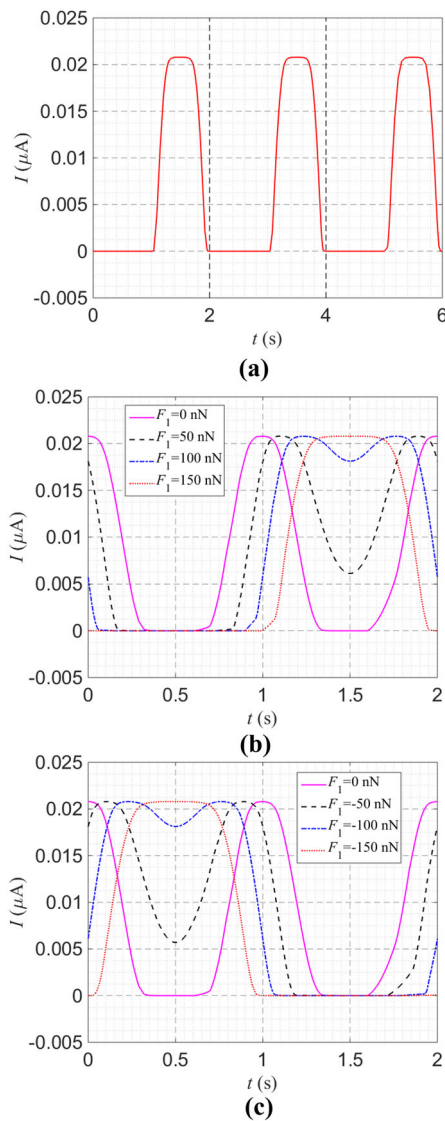


Fig. 3. Current I in the fiber versus time t under $F = F_0 \cdot \sin(\omega t) + F_1$: **a** $F_1 = 150$ nN, $\omega = \pi$ and $F_0 = 150$ nN; **b** $F_1 > 0$, $\omega = \pi$ and $F_0 = 150$ nN; **c** $F_1 < 0$, $\omega = \pi$ and $F_0 = 150$ nN

3. Numerical Results and Discussion

Specifically, consider an n-type ZnO fiber with $p \cong 0$. We denote $n_0 = N_D^+$ and use $n_0 = 10^{21} \text{ m}^{-3}$ in our calculations below. $L = 3000 \text{ nm}$. $a = 60 \text{ nm}$. The circular cross-sectional area is $A = 2.6 \times 10^{-15} \text{ m}^2$ with a radius of $R = 28.75 \text{ nm}$. $V = 1.5 \text{ volt}$ is used. The material constants of ZnO are the same as those in [27].

Consider the simple case of $F = F_0 \cdot \sin(\omega t)$ first. Figure 2 shows the current $I = J^n \cdot A$ in the fiber versus time t . Figure 2a shows the most basic result of this paper, i.e., the time-harmonic F leads to pulse currents in the fiber. This is not surprising in view of the result of [26] that a properly applied F may act like a switch that can turn the current on and off. Figure 2b shows that the frequency of the pulses is determined by ω , which is as expected. Figure 2c shows that as F_0 increases, the pulses become narrower and steeper. Numerical results also show that if F_0 is below a certain value, it does not produce pulse currents.

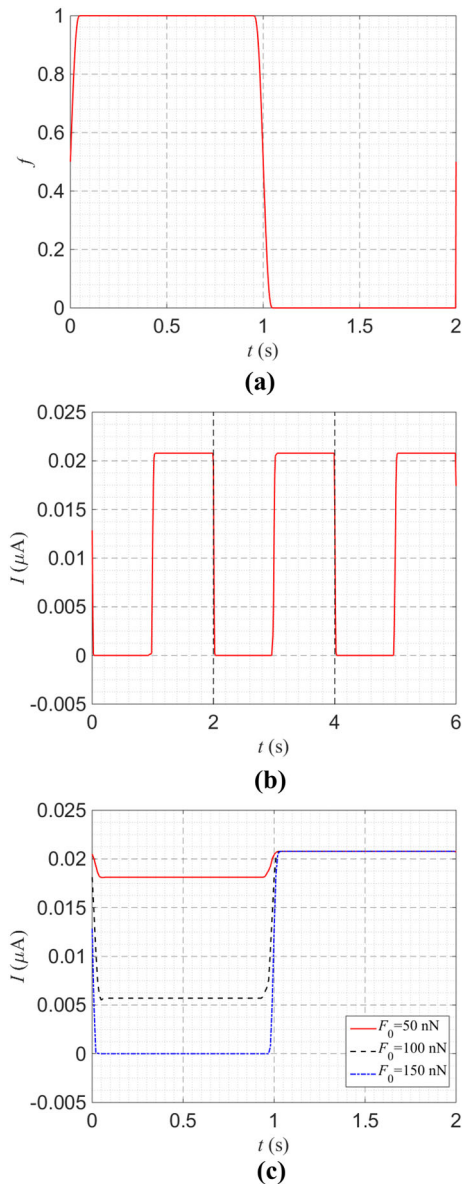


Fig. 4. Current I versus time t under $F = F_0 \cdot f(t)$, where $f(t)$ is a rectangular pulse function: a pulse function generated by COMSOL; b pulse currents when $F_0 = 150 \text{ nN}$; c effect of F_0

Next, we consider stresses described by $F = F_0 \cdot \sin(\omega t) + F_1$, with a constant part described by F_1 . The result is shown in Fig. 3. Again, Fig. 3a shows that pulse currents are produced, but the number of pulses is about half of that in Fig. 2a during the same initial six seconds. This is because the numerical values used for F_1 and F_0 are equal, and the local stress field produced by F has only three peaks during six seconds. Figure 3b, c shows that the pulse currents are sensitive to the parameters. For certain combinations of the parameters, F does not produce neat pulses.

The pulse currents in Figs. 2 and 3 are abrupt at the bottom and gradual at the top. This is related to the trigonometric F used, which is gradual. To achieve square pulse currents, we try $F = F_0 \cdot f(t)$, where $f(t)$ is a rectangular pulse function created by COMSOL numerically, as shown in Fig. 4a. Only one period is shown in Fig. 4a, which is then extended periodically. In this case, Fig. 4b shows that the currents are also square pulses. Figure 4c shows the effect of F_0 . It can be seen that the amplitude of the pulse current can be tuned by F_0 .

4. Conclusions

It is shown through a one-dimensional macroscopic model and numerical analysis by COMSOL that local time-harmonic or periodic stresses produce pulse currents in a piezoelectric semiconductor fiber under a constant voltage. The pulse currents are sensitive to the parameters of the local stresses. This offers a new approach for the mechanical manipulation of electrical behaviors of piezoelectric semiconductor fibers and may be useful in piezotronic and piezo-phototronic devices.

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