Transient Bending Vibration of a Piezoelectric Semiconductor Nanofiber under a Harmonic Shear Force

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Abstract. A harmonic shear end force induced the transient bending vibration is analyzed in a cantilevered n-type ZnO nanofiber. Based on the mechanical movement equation, continuity condition of current density and charge equation of electrostatics, the theoretical analysis is carried out by a one-dimensional model. The evolution of the deflection and perturbation of the electron concentration caused by the harmonic end force are calculated. Numerical results show that the vibration period of the piezoelectric semiconductor fiber is about twice that of the harmonic force, which referenced to design the nanosensors and nanogenerators.

1. Introduction
Piezoelectric semiconductor are widely used in many fields, which can convert mechanical energy into electricity, or vice versa. Among all methods, piezoelectric nanogenerators is one of the most convenient to convert mechanical energy into electricity. Nanowires (NWs) like ZnO, GaN, and ZnS are the most popular materials for nanogenerators, and among which, ZnO is the one we discussed in this paper. As we all know, piezoelectric semiconductor nanowires have already been reported for converting mechanical energy into electricity [1-2]. Besides, when there is an elastic wave propagates in a piezoelectric semiconductors, a electric field will be stimulate to drive carriers into motion, and on the other hand, the movement of carriers will produce some influences on electric field in turn. It indicates that many new microelectronic devices with modern functions can be developed by this interaction, like piezoelectric field-effect transistors[3-8], piezoelectric charge-coupled devices[9-12], and piezoelectric chemical sensors[13-14], etc.

Knowledge on the static, transient, and time-harmonic behaviors of piezoelectric conductor are important to their operation [15]. Extensional [16-18], flexural [19-24] and even the time-harmonic behaviors of nanowires have been already studied before.

However, few reports on transient processes are presented in recently years except transient extensional vibrations in a ZnO fiber caused under an end force [25] and transient bending vibrations by a suddenly applied shear end force [26]. In this paper, we will study the transient process of a cantilevered n-type ZnO nanofiber with a suddenly harmonic shear force in the free end. Numerical results will be presented and analyzed in the following.

2. One-dimensional Equations for the Transient Bending
A cantilevered fiber with arbitrary cross section of which the area to be A is considered in this case shown in Fig.1, and besides the length is much larger than the cross section. When t=0, a harmonic shear force $f_y = F \sin(\omega t)$ with $F = 0.2\text{nN}$ and $\omega = 1\text{GHz}$ suddenly acts on the free end. For simplicity, a crystal of class 6mm is easy to calculated and we will take this into account.
mechanical movement equation, charge equation of electrostatics and continuity condition of current density are

\[
\frac{\partial T_3}{\partial x_3} = \rho \ddot{u}_3, \\
\frac{\partial D_3}{\partial x_3} = -q \Delta n, \\
q \frac{\partial}{\partial t} (\Delta n) = \frac{\partial J_3^n}{\partial x_3}.
\]

(1)

where \( T_3 \) is the axial stress, \( u_3 \) the displacement, \( \rho \) the mass density, \( q \) electronic charge, \( D_3 \) the electric displacement, \( J_3^n \) the electron current density, and \( \Delta n \) the carrier concentration perturbation.

The relevant one-dimensional constitutive relations are \([12]\)

\[
T_3 = \overline{c}_{33} S_3 - \overline{\epsilon}_{33} E_3, \\
D_3 = \overline{\epsilon}_{33} S_3 + \overline{c}_{33} E_3, \\
J_3^n = q n_0 \mu_3^n E_3 + q D_3^{\phi} \frac{\partial (\Delta n)}{\partial x_3}.
\]

(2)

where \( E_3 \) and \( S_3 \) are the electric field and the strain, \( \mu_3^n \) and \( D_3^{\phi} \) the mobility constant and the diffusion constant. \( \overline{c}_{33} \), \( \overline{\epsilon}_{33} \) and \( \overline{c}_{33} \) are the modified elastic, piezoelectric and dielectric constants which can be defined through \([25]\). In addition, the mechanical strain and piezoelectric field can be expressed by displacement and electric potential

\[
S_3 = \frac{\partial u_3}{\partial x_3},
\]

\[
E_3 = -\frac{\partial \varphi}{\partial x_3}.
\]

(3)

For the bending of a piezoelectric semiconductor fiber in this case, we use the one-dimensional theory \([26]\). In this theory, the mechanical displacements, electric potential, and electron concentration perturbation relevant to bending of n-type piezoelectric semiconductor can be approximated by:

\[
u_2(x_3,t) \equiv v(x_3,t), \\
u_1(x_3,t) \equiv x_3 \psi(x_3,t), \\
\varphi(x_3,t) \equiv x_3 \phi^{(1)}(x_3,t), \\
\Delta n(x_3,t) \equiv x_3 n^{(1)}(x_3,t),
\]

(4)

where \( v(x_3,t) \) and \( \psi(x_3,t) \) are the deflection and the shear deformation related to bending. The
motion equations, the charge equation of electrostatics and the conservation of charge for electrons are as follows \[26\]

\[
Q = \rho A \dot{v},
\]

\[
M_{1,3} - Q = \rho I \dot{\psi},
\]

\[
D_{1,3}^{(1)} - D_2^{(0)} = qI(-n^{(1)}),
\]

\[
J_3^{n(1)} - J_2^{n(0)} = qIn^{(1)},
\]

where \(I\) and \(A\) are the moment of inertia and the area of the cross section of the fiber. The bending moment \(M_1\), the transverse shear force \(Q\), the zero- and first-order moments of the relevant electric displacement and current components are \[26\]

\[
M_1 = \int_A x_T dA = \overline{\varepsilon}_{33} I v_{3,3} + \overline{\varepsilon}_{33} I \phi_3^{(1)},
\]

\[
Q = \int_A T_v dA = \overline{\varepsilon}_{44} A (v_{3,3} + \psi) + \overline{\varepsilon}_{44} A \phi_3^{(1)},
\]

\[
D_2^{(0)} = -\overline{\varepsilon}_{11} A \phi^{(1)},
\]

\[
D_3^{(1)} = -\overline{\varepsilon}_{33} I v_{3,3} - \overline{\varepsilon}_{33} I \phi_3^{(1)},
\]

\[
J_2^{(0)} = \int_A J_2^0 dA = -q n_{0,3} \mu_{0,1} A \phi^{(1)} + qD_{1,1}^{n(1)} A n^{(1)},
\]

\[
J_3^{n(1)} = \int_A x_2 J_3^0 dA = -q n_{0,3} \mu_{0,1} I \phi_3^{(1)} + qD_{1,3}^{n(1)} I n^{(1)}.
\]

The above equations are for bending vibration with shear deformation. In addition, we assume that bending without shear deformation, so we get expression in the following

\[
\psi = -v_3.
\]

Then (6) and (7) reduce to

\[
M_1 = -\overline{\varepsilon}_{33} I v_{3,3} + \overline{\varepsilon}_{33} I \phi_3^{(1)},
\]

\[
D_2^{(0)} = -\overline{\varepsilon}_{11} A \phi^{(1)},
\]

\[
D_3^{(1)} = -\overline{\varepsilon}_{33} I v_{3,3} - \overline{\varepsilon}_{33} I \phi_3^{(1)}.
\]

In bending without shear, the moment of inertia \(I\) on the right-hand side of (5)_2 can be neglected. Then (5)_2 can be simplified that

\[
Q = M_{1,3} = -\overline{\varepsilon}_{33} I v_{3,33} + \overline{\varepsilon}_{33} I \phi_3^{(1)}.
\]

Effectively, (12) serves as the constitutive relation for \(Q\) which, when substituted into (5)_1, yields the equation for bending without shear:

\[
-\overline{\varepsilon}_{33} I v_{3,33} + \overline{\varepsilon}_{33} I \phi_3^{(1)} = \rho A \dot{v}.
\]

The substitution of (11) into (5)_3 yields

\[
-\overline{\varepsilon}_{33} I v_{3,33} - \overline{\varepsilon}_{33} I \phi_3^{(1)} + \overline{\varepsilon}_{11} A \phi^{(1)} = qI(-n^{(1)}).
\]

The substitution of (8) into (5)_4 gives

\[
-n_{0,3} \mu_{0,1} I \phi_3^{(1)} + D_{33}^{n(1)} I n^{(1)} + n_{0,3} \mu_{0,1} A \phi^{(1)} - D_{33}^{n(1)} A n^{(1)} = In^{(1)}.
\]

(13)-(15) are the three equations needed for \(v, \phi^{(1)},\) and \(n^{(1)}\).
3. Numerical Results and Discussion

According to [26], the length and radius of the ZnO nanofiber which we consider is 600nm and 25nm. The initial carrier concentration is \( n_0 = 10^{23} \text{ m}^{-3} \), the mass density \( \rho = 5606 \text{ kg/m}^3 \), and related coefficients are as follows,

\[
(c_{11}, c_{12}, c_{13}, c_{33}, c_{44}) = (207, 117.7, 106.1, 209.5, 44.8) \text{ GPa},
\]

\[
(e_{31}, e_{33}, e_{15}) = (-0.51, 1.22, -0.45) \text{ C/m}^2, \quad (e_{11}, e_{33}) = (7.77, 8.91) \epsilon_0, \quad (16)
\]

\[
\kappa_{33}^n = 5.2 \times 10^{-4} \text{ m}^2/\text{s}, \quad \mu_{33}^n = 0.02 \text{ m}^2/\text{Vs}.
\]

Right after the load is applied to the free end, the fiber rises from the initial state with a zero deflection, gradually reaches its largest deflection, and then falls back to essentially a zero deflection, after that reverse increase to maximum deflection, and falls back to zero deflection again, which is called a period approximately. The deflection \( L \) along the fiber disturbed by the suddenly harmonic shear ending force is analyzed at different time instants shown in Fig.2. As the shear force acts on the fiber, different kinds of waves will be generated, long waves propagate slowly and short waves propagate quickly, so when the shear force is applied, the right side will immediately deform. We notice that the maximum deflection is different, that is because the shear force is different at different time instant, which influences the value of deflection. Besides, the vibration period of the piezoelectric semiconductor fiber is approximately twice that of the harmonic force.

![Figure 2. Deflection curves of the fibers at different time instants](image)

In Fig. 3 \( \Delta n = x_2 n^{(1)}(x_3, t) \) at four time instants are shown during the first period of the motion. Figure 4(a) and 4(c) shows the electron distribution when there are the largest forward deflection and reverse deflection, however, the largest change of \( \Delta n \) happens at the left end but we do not show it. In these cases, \( \Delta n \) is linear in \( x_2 \), with more electrons at the top surface and less at the bottom surface, besides, the amplitude of the distribution is more than twice that of the static case in [26]. And also, we find that no matter when the deflection comes to zero, the electrons form a distribution that does not change much along the fiber than the case when there is a deflection. The small oscillations do not seem to affect the overall qualitative picture of the distribution.
Figure 3. Electron concentration perturbation \( \Delta n = x_n n^{(1)}(x, t) \) in \( L/6 < x < L \) at four different
time instants. (a) \( t = 4.27 \) ns. a) \( t = 5.73 \) ns. (c) \( t = 8.27 \) ns. (d) \( t = 10.0 \) ns.

4. Conclusions
Transient vibration of a ZnO fiber is analyzed under a suddenly harmonic shear ending force.
One-dimensional theory is used in this article and deflection are solved. As the shear ending force is
different at different time instant, so the time of deflection change is inconsistent. Later, the
distribution of carriers are shown at four special time instants. Finally, present results can be
referenced to design the nanosensors and nanogenerators.

5. References
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