University of Nebraska - Lincoln

DigitalCommons@University of Nebraska - Lincoln

Mechanical & Materials Engineering Faculty Publications

Mechanical & Materials Engineering, Department of

2016

Propagation of extensional waves in a piezoelectric semiconductor rod

C.L. Zhang
Zhejiang University, Hangzhou

X. Y. Wang
Zhejiang University, Hangzhou

W. Q. Chen
Zhejiang University, Hangzhou

J. S. Yang
Zhejiang University, Hangzhou

Follow this and additional works at: http://digitalcommons.unl.edu/mechengfacpub

Part of the Mechanics of Materials Commons, Nanoscience and Nanotechnology Commons, Other Engineering Science and Materials Commons, and the Other Mechanical Engineering Commons

Propagation of extensional waves in a piezoelectric semiconductor rod

C.L. Zhang,[1,2,3,a] X. Y. Wang,[1] W. Q. Chen,[1,2,3] and J. S. Yang[1,4]

[1]*Department of Engineering Mechanics, Zhejiang University, Hangzhou, 310027, China*
[2]*Soft Matter Research Center (SMRC), Zhejiang University, Hangzhou 310027, P.R. China*
[3]*Key Laboratory of Soft Machines and Smart Devices of Zhejiang Province,*
Hangzhou 310027, P.R. China
[4]*Department of Mechanical and Materials Engineering, University of Nebraska-Lincoln,*
Lincoln, NE 68588-0526, USA

We studied the propagation of extensional waves in a thin piezoelectric semiconductor rod of ZnO whose *c*-axis is along the axis of the rod. The macroscopic theory of piezoelectric semiconductors was used which consists of the coupled equations of piezoelectricity and the conservation of charge. The problem is nonlinear because the drift current is the product of the unknown electric field and the unknown carrier density. A perturbation procedure was used which resulted in two one-way coupled linear problems of piezoelectricity and the conservation of charge, respectively. The acoustic wave and the accompanying electric field were obtained from the equations of piezoelectricity. The motion of carriers was then determined from the conservation of charge using a trigonometric series. It was found that while the acoustic wave was approximated by a sinusoidal wave, the motion of carriers deviates from a sinusoidal wave qualitatively because of the contributions of higher harmonics arising from the originally nonlinear terms. The wave crests become higher and sharper while the troughs are shallower and wider. This deviation is more pronounced for acoustic waves with larger amplitudes. © *2016 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/).* [http://dx.doi.org/10.1063/1.4945752]

I. INTRODUCTION

Piezoelectric materials are widely used to make electromechanical transducers for converting electric energy to mechanical energy or vice versa, and acoustic wave devices for frequency operation and sensing. In most cases, piezoelectric crystals and ceramics are treated as nonconducting dielectrics but in reality there is no sharp division separating conductors from dielectrics. Real materials more or less have some conduction.[1] For example, in acoustic wave devices made from quartz crystals, the small ohmic conduction and the related dissipative effects need to be considered when calculating the Q value (quality factor) of the devices[2–4] because other dissipative effects in quartz such as material damping and radiation damping are very small. Another origin of conduction in piezoelectric crystals is that some of them are in fact semiconductors with charge carriers of electrons and/or holes,[5] e.g., the widely used ZnO and AlN films and fibers. In these materials, in addition to carrier drift under an electric field, carrier diffusion also contributes to the electric current in the material. Piezoelectric semiconductors have been used to make devices for acoustic wave amplification[6–9] and acoustic charge transport[10,11] based on the acoustoelectric effect, i.e., the motion of carriers under the electric field produced by an acoustic wave through piezoelectric coupling. Recently, the electric field produced by mechanical fields in a piezoelectric semiconductor has been used to manipulate the operation of semiconductor devices, which forms the foundation

---

[a]corresponding author: Dr. Chunli Zhang, E-mail: zclwei@zju.edu.cn

of piezotronics.[12–14] Piezoelectric semiconductors such as ZnO are also used for mechanical energy harvesting and conversion to electric energy.[15–18]

The basic behaviors of piezoelectric semiconductors can be described by the conventional theory consisting of the equations of linear piezoelectricity and the equations for the conservation of charge for electrons and holes (the continuity equations).[19] This theory has been used to study some of the applications in the above, the inclusion problem for piezoelectric semiconductor composites,[20] the fracture of piezoelectric semiconducting materials,[21–23] the electromechanical energy conversion in these materials,[24] vibrations of piezoelectric semiconductor plates,[25] and to develop low-dimensional theories of piezoelectric semiconductor plates and shells.[26,27] Researchers have also developed more general and fully nonlinear theories for piezoelectric semiconductors under strong electric fields with large mechanical deformations.[28–30]

This paper is concerned with the propagation of extensional waves in a thin piezoelectric semiconductor rod which is often used in piezoelectric semiconductor devices. This problem is fundamental to the applications of piezoelectric semiconductor rods or wires. The theoretical formulation is for small amplitude waves governed by the linear theory of piezoelectricity but the problem is still nonlinear because the drift current is proportional to the product of the unknown carrier density and the unknown electric field,[31] which presents mathematical challenges. We performed a theoretical analysis using a one-dimensional model developed in our previous static analysis of a piezoelectric semiconductor rod.[32] An approximate solution was obtained showing a few nonlinear aspects of the wave.

II. ONE-DIMENSIONAL MODEL FOR A ROD

Consider a cylindrical piezoelectric semiconducting rod which, along with its coordinate system, is shown in Fig. 1. The cross section of the rod is arbitrary. Its surface is traction free. The rod is made from crystals of class 6 mm such as ZnO. The c-axis of the crystal is along the axis of the rod, i.e., the x_3 axis. The rod is assumed to be long and thin. The electric field in the surrounding free space is neglected.

For extensional waves in a thin rod, the deformation is mainly the axial strain accompanied by lateral strains due to Poisson's effect which can be described by a one-dimensional model.[32] The governing equations are the linear momentum equation, the charge equation of electrostatics, and the conservation of electrons and holes:
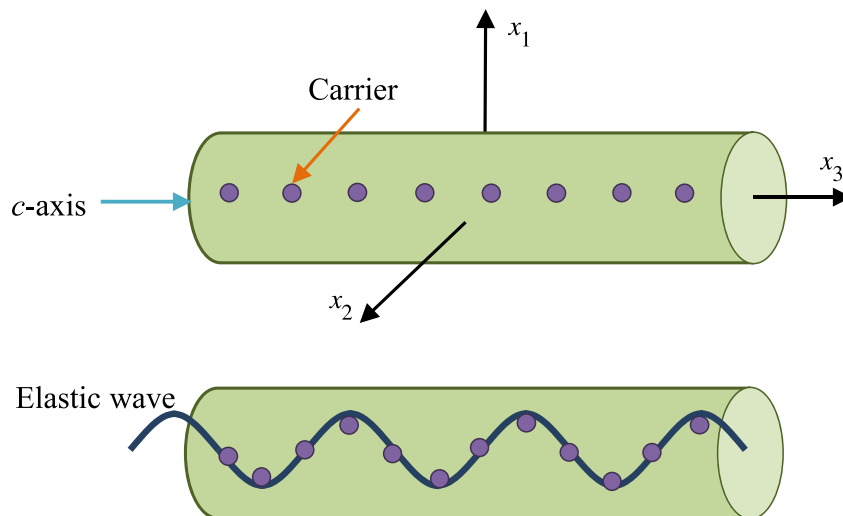

FIG. 1. The sketch of a piezoelectric semiconductor rod of crystals of 6 mm that is uniformly doped (top) and the elastic wave coupled with the motion of carriers (bottom).

$$
\begin{aligned}
T_{3,3} &= \rho \ddot{u}_3, \\
D_{3,3} &= q(p - n + N^+ - N^-), \\
J^n_{3,3} &= q\dot{n}, \\
J^p_{3,3} &= -q\dot{p},
\end{aligned}
\tag{1}
$$

where T_3 is the axial stress, ρ the mass density, u_3 the axial displacement, D_3 the axial electric displacement, $q = 1.6 \times 10^{-19}$ coul the electronic charge, p and n the densities of holes and electrons, N^+ and N^- the densities of impurities of donors and accepters, and J^p_3 and J^n_3 the axial hole and electron current densities. We are interested in the motion of the existing carriers in the rod driven by the electric field associated with an acoustic wave. Therefore, in (1) we have neglected the effect of the acoustic wave on energy bands and the carrier recombination and generation.[6,19] The Cartesian tensor notation and the compact matric notation for tensor indices have been used. A comma followed by an index indicates a partial derivative with respect to the coordinate associated with the index. A superimposed dot represents a time derivative. We consider uniformly doped n-type semiconductors for which n and N^+ are much greater than p and N^-. Therefore, we neglect p and N^- in (1). In this case $(1)_{1-3}$ become uncoupled to the p in $(1)_4$ which will be dropped in the following. Constitutive relations for the relevant axial fields in $(1)_{1-3}$ are

$$
\begin{aligned}
T_3 &= \bar{c}_{33} S_3 - \bar{e}_{33} E_3, \\
D_3 &= \bar{e}_{33} S_3 + \bar{\varepsilon}_{33} E_3, \\
J_3 &= qn\mu_{33} E_3 + qD_{33} n_{,3},
\end{aligned}
\tag{2}
$$

where $J_3 = J^n_3$, D_{33} the electron diffusion coefficient, and the effective one-dimensional elastic, piezoelectric, and dielectric constants obtained by the stress relaxation conditions $T_1 = T_2 = 0$ are given by

$$
\begin{aligned}
\bar{c}_{33} &= 1/s_{33}, \\
\bar{e}_{33} &= d_{33}/s_{33}, \\
\bar{\varepsilon}_{33} &= \varepsilon_{33} - d_{33}^2/s_{33},
\end{aligned}
\tag{3}
$$

where s_{33} is the compliance constant, d_{33} the piezoelectric constant, and ε_{33} the dielectric constant. The mobility and the diffusion constant in $(2)_3$ are related by the Einstein relationship[31]

$$
\frac{\mu_{33}}{D_{33}} = \frac{q}{kT}.
\tag{4}
$$

The relevant strain-displacement relation as well as the electric field-potential relation are

$$
\begin{aligned}
S_3 &= u_{3,3}, \\
E_3 &= -\phi_{,3}.
\end{aligned}
\tag{5}
$$

With the use of (5), (2) becomes

$$
\begin{aligned}
T_3 &= \bar{c}_{33} u_{3,3} + \bar{e}_{33} \phi_{,3}, \\
D_3 &= \bar{e}_{33} u_{3,3} - \bar{\varepsilon}_{33} \phi_{,3}, \\
J_3 &= -qn\mu_{33} \phi_{,3} + qD_{33} n_{,3},
\end{aligned}
\tag{6}
$$

which are the one-dimensional constitutive relations ready to be used in $(1)_{1-3}$.

The substitution of (6) into $(1)_{1-3}$ yields

$$
\begin{aligned}
\bar{c}_{33} u_{3,33} + \bar{e}_{33} \varphi_{,33} &= \rho \ddot{u}_3, \\
\bar{e}_{33} u_{3,33} - \bar{\varepsilon}_{33} \varphi_{,33} &= q(N^+ - n), \\
-\mu_{33}\varphi_{,33} n - \mu_{33}\varphi_{,3} n_{,3} + D_{33} n_{,33} &= \dot{n}.
\end{aligned}
\tag{7}
$$

(7) has three equations for u_3, φ, and n.

III. PROPAGATION OF EXTENSIONAL WAVES

The displacement u_3, electric potential φ and carrier density n are coupled together in (7), and the first two terms in (7)$_3$ are nonlinear. This makes (7) mathematically complicated and challenging. As the property of carrier motion in piezoelectric semiconductor rod under an elastic wave is our concern in this paper. For simplicity, we only consider the case of low carrier densities and neglect the effect on elastic wave from carriers. Consequently, we can make an approximation by dropping the charges $q(N^+ - n)$ on the right-hand side of (7)$_2$, and (7) is reduced to two one-way coupled systems of

$$\bar{c}_{33}u_{3,33} + \bar{e}_{33}\varphi_{,33} = \rho\ddot{u}_3,$$
$$\bar{e}_{33}u_{3,33} - \bar{\varepsilon}_{33}\varphi_{,33} = 0, \qquad (8)$$

and

$$-\mu_{33}\varphi_{,33}n - \mu_{33}\varphi_{,3}n_{,3} + D_{33}n_{,33} = \dot{n}. \qquad (9)$$

This can be viewed as the lowest order of approximation in a perturbation procedure using $q(N^+ - n)$ as a small parameter.

(8) is the classical theory of piezoelectricity for which extensional waves in the rod in Fig. 1 are described by

$$u_3 = A\cos\psi, \quad \varphi = B\cos\psi, \qquad (10)$$

where

$$\psi = \xi x_3 - \omega t, \quad \omega^2 = \frac{c_{33}^*}{\rho}\xi^2,$$
$$c_{33}^* = \bar{c}_{33} + \frac{\bar{e}_{33}^2}{\bar{\varepsilon}_{33}}, \quad B = \frac{\bar{e}_{33}}{\bar{\varepsilon}_{33}}A. \qquad (11)$$

In (11), ξ is the wave number, A and B are the amplitudes of the displacement and electric potential, respectively. The electric field accompanying the waves in (10) is $E = B^*\sin\psi$, and $B^* = A\xi\bar{e}_{33}/\bar{\varepsilon}_{33}$. With the electric potential given in (10), (9) becomes

$$\xi\mu_{33}\cos\psi B^* n + \mu_{33}\sin\psi B^* n_{,3} + D_{33}n_{,33} = \dot{n}, \qquad (12)$$

which is linear for n. However, it has variable coefficients depending on both x_3 and t through φ and is still a mathematically challenging problem. We can write the carrier density, which is the solution to (12), using the following Fourier series

$$n(x_3,t) = a_0 + \sum_{m=1}^{M}\left(a_m\cos m\psi + b_m\sin m\psi\right). \qquad (13)$$

where a_0, a_m and b_m are coefficients which are independent of space and time. As in Ref. 19, we may write the carrier density (13) in the form of

$$n = n_0 + n_d, \qquad (14)$$

where $n_0 = a_0$ and

$$n_d = \sum_{m=1}^{M}\left(a_m\cos m\psi + b_m\sin m\psi\right). \qquad (15)$$

(14) or (13) shows that the carrier density $n(x_3,t)$ in the rod includes a uniform static part n_0 which is the mean density, and a dynamic part $n_d(x_3,t)$. From (14), the carrier density at $t = 0$ is $n(x_3,0) = n_0 + \sum_{m=1}^{M}(a_m\cos m\xi x_3 + b_m\sin m\xi x_3)$. In fact, $n(x_3,0)$ is just the carrier density in the equilibrium state without elastic wave motion. For a uniformly doped rod, the carrier density is independent of x_3. We immediately conclude that $n(x_3,0) = n_0$, namely, the value of the mean
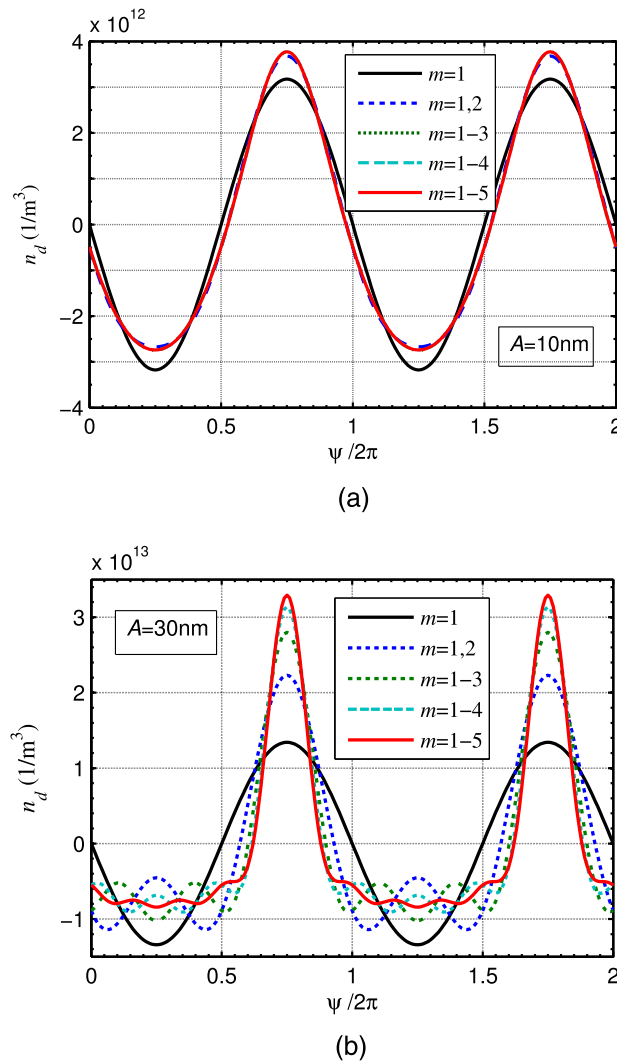
FIG. 2. n_d for different values of A, $M = 5$. (a) $A = 10$ nm. (b) $A = 30$ nm.

density n_0 under elastic wave equals the carrier density in the equilibrium state. In (15) the unknown constants a_m and b_m can be determined by substituting (13) into (12). Then write both sides of the resulting equation in terms of $\cos m\psi$ and $\sin m\psi$ using trigonometric identities, and equal the corresponding coefficients. This yields a hierarchy of linear equations for a_m and b_m. The accuracy of the solution of (14) depends on the truncated term M.

Next, we consider that the deviation n_d is very small. Substituting (14) into (12), we obtain the following equation for n_d:

$$\dot{n}_d = \mu_{33}B^*\xi \cos\psi\, n_0 + \mu_{33}B^*\xi \cos\psi\, n_d + \mu_{33}B^* \sin\psi\, n_{d,3} + D_{33}n_{d,33}. \tag{16}$$

The first three terms on the right-hand side of (16) are from the nonlinear drift current, and the last term is from the diffusion current. The first term $\mu_{33}B^*\xi \cos\psi\, n_0$ does not depend on n_d and is effectively a driving term by the wave in (10). As n_d is very small, only the first term on right-hand side of (16) is kept. Consequently, the solution to (16) is

$$n_d = -\mu_{33}n_0 B^* \frac{\xi}{\omega} \sin\psi. \tag{17}$$

(17) describes a simple sinusoidal wave motion of the carriers driven by the electromechanical wave in (10). The solution (17) is only a special case of the solution (15).
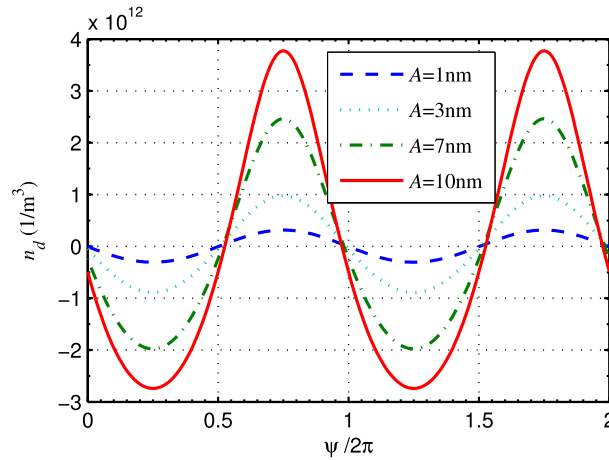
(a)
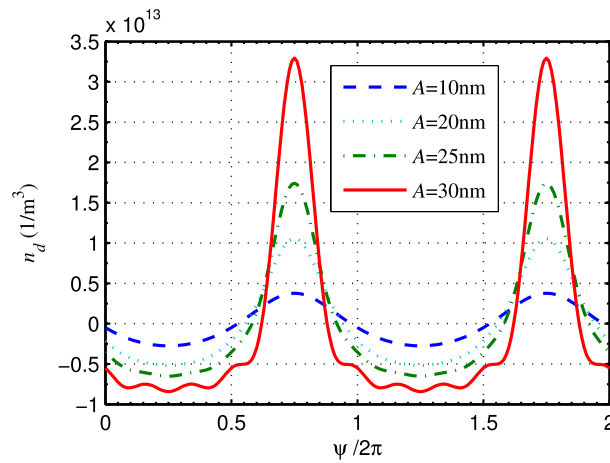
(b)

FIG. 3. Effect of the wave amplitude A in (10).

IV. NUMERICAL RESULTS AND DISCUSSION

The elastic, dielectric and piezoelectric constants for ZnO can be found in Ref. 5. At room temperature $kT/q = 0.026$ V.[31] $\mu_{33} = 0.015$ m^2/V · s. Here, the electron density in equilibrium condition $n_0 = 10^{13}$ 1/m^3 was used. Consider a rod with a cross sectional dimension characterized by some diameter $d = 1$ mm. For a wave with wavelength $\lambda = 10$ mm which is much larger than the cross sectional dimension for the one-dimensional model to be valid, the wave number $\xi = 2\pi/\lambda = 628.3$ 1/m. Then from (11) the wave frequency is $\omega = 3.49 \times 10^6$ 1/s. The wave amplitude A will be varied in the computation. In the case when the amplitude $A = 10$ nm (and 30 nm), the corresponding amplitude of the axial strain $S_3 = u_{3,3}$ is $A\xi = 6.283 \times 10^{-6}$ (and 18.85×10^{-6}).

For the extensioanl wave with amplitude $A = 10$ nm, we use $M = 5$ in (14) and compute the corresponding coefficiencts a_m and b_m ($m = 1, 2, 3, 4, 5$). Fig. 2(a) are curves of the carrier density n_d with retaining $m = 1$, $m = 1$ and 2, $m = 1$-3, $m = 1$-4, and $m = 1$-5 terms in (14), respectively. The case of using $m = 1$ and 2 and the case of using $m = 1$-5 terms are almost identical, showing the rapid convergence of the series. The wave is periodic. Therefore only two periods are shown. The black solid line corresponding to using $m = 1$ only is a sinusoidal wave. Once the higher-order terms with $m = 2$ or larger are included, the wave is no longer sinusoidal. The crests become higher and narrower, and the troughs shallower and wider. These do not happen in a linear system and is
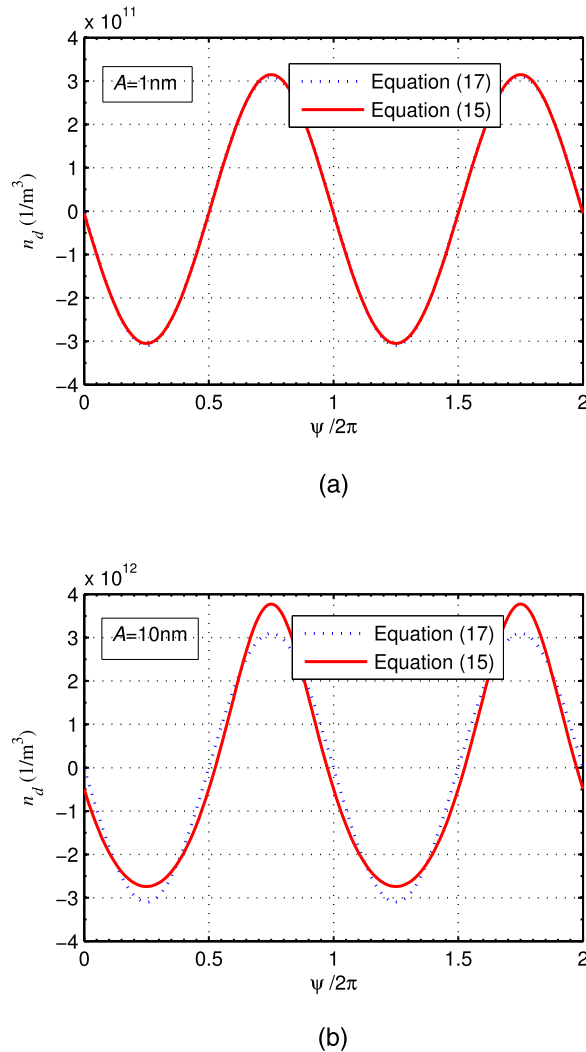
(a)

(b)

FIG. 4. Comparison of (15) and (17).

believed to be caused by the nonlinearity in the problem. We note that in Fig. 2(a) the amplitude of the dynamic part of the carrier density is about 4×10^{12} 1/m^3 which is less than $n_0 = 10^{13}$ 1/m^3.

In Fig. 2(b) the acoustic wave amplitude is increased to $A = 30$ nm and everything else is kept the same as in Fig. 2(a). When A is increased, the strains of the wave becomes larger and nonlinear effects are expected to be more pronounced. Not surprisingly, Fig. 2(b) shows that in this case the convergence is slower with small oscillations of the troughs, and the deviation from a sinusoidal wave is more severe. Very interestingly, the wave amplitude seems to be bounded from below. The depth of the troughs is approximately 10^{13} 1/m^3, the same as n_0 and thus the total carrier density of $n_0 + n_d$ remains nonnegative.

The deviation from a sinusoidal wave is believed to be due to the nonlinearity in the problem. Nonlinearity is associated with large mechanical deformations and strong electric fields. Fig. 2 suggests that as the amplitude of the wave, A, in (10) increases, the deviation from a sinusoidal wave is more pronounced. To examine this more closely we calculate n_d for increasing values of A in the range from 1nm to 30 nm with $M = 5$. The results are summarized in Figs. 3(a) and 3(b). In Fig. 3(a), when A is small, the wave is essentially sinusoidal. As A increases, deviation from a sinusoidal wave becomes visible. The height of the crests is larger than the depth of the troughs, and the crests are narrower than the troughs. As A increases further in Fig. 3(b), the wave deviates from a sinusoidal one severely.

From Fig. 2(a) and Fig. 3(a), the wave seems to be sinusoidal when the wave amplitude A is small. The curve described by $m = 1$ in Fig. 2(a) in fact has both a sine and a cosine term in (15) when $m = 1$. We suspect that in fact the sine term given in (17) is the dominating term for small amplitude waves. To demonstrate this we plot the single term in (17) versus the series in (15) with $M = 5$ in Fig. 4 for two different values of the wave amplitude. In Fig. 4(a), the two curves are indistinguishable. Clearly, for small A, the wave is nearly sinusoidal and (17) is a good approximation.

V. SUMMARY

In a piezoelectric semiconductor rod of ZnO with the c-axis along the axis of the rod, the extensional wave produces an axial electric field which causes axial motions of carriers. The governing equations are nonlinear because of the drift motion of carriers. When the extensional wave is approximately linear and sinusoidal, the wave motion of the carriers is not sinusoidal. The crests become higher and narrower while the troughs are shallower and wider. This deviation from a sinusoidal wave is more pronounced when the amplitude of the extensional wave increases which is associated with larger strains and stronger electric fields. The dynamic part of the carrier density seems to be bounded from below so that the total density is nonnegative.

ACKNOWLEDGMENTS

[1] H.F. Tiersten and T.-L. Sham, IEEE Trans. Ultras. Ferroelectr. Freq. Contr. **45**, 1 (1998).
[2] Y-K. Yong, M.S. Patel, and M. Tanaka, IEEE Trans. Ultras. Ferroelectr. Freq. Contr. **57**, 1831 (2010).
[3] P.C.Y. Lee, N.H. Liu, and A. Ballato, Trans. Ultras. Ferroelectr. Freq. Contr. **51**, 52 (2004).
[4] J. Wang, W.H. Zhao, J.K. Du, and Y.T. Hu, Ultrasonics **51**, 65 (2011).
[5] B.A. Auld, *Acoustic Fields and Waves in Solids* (John Wiley and Sons, New York, 1973), Vol. I.
[6] D.L. White, J. Appl. Phys. **33**, 2547 (1962).
[7] J.S. Yang and H.G. Zhou, Acta Mechanica **172**, 113 (2004).
[8] S.K. Ghosh, Indian J. Pure Appl. Phys. **44**, 183 (2006).
[9] M. Willatzen and J. Christensen, Phys. Rev. B **89**, 041201 (2014).
[10] F.J.R. Schulein, K. Muller, M. Bichler *et al.*, Phys. Rev. B **88**, 085307 (2013).
[11] S. Buyukkose, A. Hernandez-Minguez, B. Vratzov *et al.*, Nanotech. **25**, 135204 (2014).
[12] X.D. Wang, J. Zhou, J.H. Song *et al.*, Nano Lett. **6**, 2768 (2006).
[13] Z.L. Wang, Adv. Mater. **19**, 889 (2007).
[14] Z.L. Wang, Nano Today **5**, 540 (2010).
[15] O. Graton, G. Poulin-Vittrant, L.T.H. Hue *et al.*, Adv. Appl. Ceram. **112**, 85 (2013).
[16] K. Yin, H.Y. Lin, Q. Cai *et al.*, Nanoscale **5**, 12330 (2013).
[17] P. Hiralal, H.E. Unalan, and G.A. Amaratunga, Nanotech. **23**, 194002 (2012).
[18] B. Kumar and S.-W. Kim, Nano Energy **1**, 342 (2012).
[19] A.R. Hutson and D.L. White, J. Appl. Phys. **33**, 40 (1962).
[20] J.S. Yang, Y.C. Song, and A.K. Soh, Arch. Appl. Mech. **76**, 381 (2006).
[21] Y.T. Hu, Y. Zeng, and J.S. Yang, Int. J. Solids Struct. **44**, 3928 (2007).
[22] J. Sladek, V. Sladek, E. Pan *et al.*, CMES **99**, 273 (2014).
[23] J. Sladek, V. Sladek, E. Pan *et al.*, Eng. Fract. Mech. **126**, 27 (2014).
[24] P. Li, F. Jin, and J.S. Yang, Smart Mater. Struct. **24**, 025021 (2015).
[25] J. Wauer and S. Suherman, Int. J. Eng. Sci. **35**, 1387 (1997).
[26] J.S. Yang and H.G. Zhou, Int. J. Solids Struct. **42**, 3171 (2005).
[27] J.S. Yang, X.M. Yang, and J.A. Turner, J. Intellig. Mater. Syst. Struct. **16**, 613 (2005).
[28] H.G. de Lorenzi and H.F. Tiersten, J. Math. Phys. **16**, 938 (1975).
[29] M.F. McCarthy and H.F. Tiersten, Arch. Rat. Mech. Anal. **68**, 27 (1978).
[30] G. Maugin and N. Daher, Int. J. Eng. Sci. **24**, 703 (1986).
[31] R.F. Pierret, *Semiconductor Fundamentals*, 2nd ed. (Addison-Wesley, Reading, Massachusetts, 1988).
[32] C.L. Zhang, X.Y. Wang, W.Q. Chen, and J.S. Yang, J. Zhejiang Univ. – SCI. A **17**, 37 (2016).