

Nonlinear Thermoelectroelastic Simulation of III-N Devices

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Abstract—A consistent thermoelectroelastic description of piezoelectric semiconductors with finite deformation is presented. By including both kinematic and constitutive nonlinearities as well as a proper treatment of the electrostatic conditions at free surfaces, the theory allows situations with large strains to be modeled more accurately. In addition, the theory is rotationally invariant unlike the linear theory, and can therefore be applied to semiconducting MEMS structures that involve large mechanical displacements. These points are illustrated using numerical simulations of several different III-N devices of technological interest.

Keywords—piezoelectric semiconductor; finite deformation; electroelasticity; nonlinearity; GaN devices; electrostriction; nanogenerator; diffusion-drift transport.

I. INTRODUCTION

In previous work a continuum description of GaN HEMTs was presented in which diffusion-drift electron transport was fully coupled to both mechanical and thermal variables, with the former accounting for the strong piezoelectricity of the III-V materials and the latter allowing inclusion of heating effects that are often important in power devices [1]. The focus of that work was GaN HEMT failure mechanisms, and especially an investigation of the cracking phenomenon known to occur near the drain edge of stressed devices. As is typical in such analyses, in order to keep the treatment relatively straightforward and with known material parameters, it was assumed that various higher order terms associated with finite mechanical deformation could be neglected and that linear theory was therefore appropriate. But given that the strain levels in such devices can be quite high (e.g., 1 to 2% or more), the validity of this infinitesimal strain assumption must be regarded as uncertain, if not dubious. A related flaw is the lack of rotational invariance in the constitutive equations used in all earlier work that leads to errors in simulations involving large rotations (but possibly infinitesimal strains) such as occur in various MEMS devices. The purpose of the present paper is to set out the nonlinear theory needed to treat large displacement/strain situations, and then to the extent possible (e.g., since many of the nonlinear coefficients are not accurately known), apply it to various GaN device problems with the goal of assessing the sizes of the errors incurred by the linearization and the possible importance of nonlinear effects such as electrostriction. More broadly, it is hoped that this general framework for treating semiconductors with large deformations might prove useful as a tool for analyzing other practical devices where “extreme” elastic states are known to serve a variety of electronic purposes,

e.g., mobility enhancement via band structure distortion, or for MEMS devices where there is significant rotational motion.

II. FINITE DEFORMATION THEORY

When mechanical deformations cannot be regarded as infinitesimal — and so are termed *finite* — it becomes essential to develop elasticity and related theories in a manner consistent with thermodynamics and with certain principles of symmetry and invariance [2]. For electroelasticity the proper treatment was first given by Toupin in 1956 using variational methods [3], and our equations largely reduce to his in the isothermal, non-semiconducting case, although our presentation is closer in spirit to the balance law approach of Tiersten [4]. In the abbreviated discussion given herein, Cartesian coordinates are used with vectors and tensors expressed in indicial notation, and with commas denoting partial differentiation.

At a continuum level, thermoelectromechanical phenomena in a piezoelectric semiconductor are governed by partial differential equations describing the coupled interactions of electroelasticity, diffusion-drift electron transport, and heat conduction. In steady-state these equations are [1]:

$$\tau_{ij,i}^M + \tau_{ij,i}^E = 0 \quad D_{i,i} = q(N - n) \quad (1a)$$

$$J_{i,i}^n \equiv (nv_i^n)_{,i} = 0 \quad J_i^n = -n\mu_n(\varphi_{,i}^n + E_i) \quad (1b)$$

$$q_{i,i} = J_i^n(\varphi_{,i}^n + E_i) \quad (1c)$$

where τ_{ij}^M is the mechanical (Cauchy) stress, τ_{ij}^E is the electrostatic Maxwell stress, E_i is the electric field, D_i is the electric displacement, the right side of (1a)₂ is the space charge inside semiconductor regions with n being the electron density and N being a bulk charge density associated with ionized impurities, J_i^n is the electron number current density, μ_n is the electron mobility, and q_i is the heat flux. The right-side of (1c) is the Joule heating associated with the electron flow, that neither (1b)₁ nor (1c) contains a generation-recombination term means that this phenomenon has been neglected, and a term accounting for the force exerted by electron pressure on the lattice has been neglected from (1a)₁. The full set of equations in (1) obviously apply only to semiconductors; in solid insulators no electron transport is allowed, in metals only heat conduction occurs, and in the surrounding air/vacuum only the electrostatics is considered.

To complete the system in (1) it is necessary to provide constitutive equations that describe various aspects of the material response such as the relationships between stress and strain and between polarization and electric field. For problems in-

volving finite deformation it is important to formulate these constitutive equations in such a way that the responses do not change when the material undergoes rigid motion [2,3]. To this end, one needs to be more precise in describing the mechanical deformation of the material mathematically. In particular, we represent this kinematics by the usual mapping:

$$y_i = y_i(X_1, X_2, X_3, t), \quad i = 1, \dots, 3 \quad (2)$$

where the y_i (with a small letter index) give the present (or Eulerian) coordinates of the material and the X_L (with a capital letter index $L = 1, \dots, 3$) define the reference (or Lagrangian) coordinates of the material. Equation (2) expresses how the present position \mathbf{y} of a material point that was initially at \mathbf{X} evolves over time t as a result of the deformation. Assuming this behavior is “smooth” so that the function in (2) is continuous and differentiable, one can define the deformation gradient as the two-point tensor $y_{i,L} = \partial y_i / \partial X_L$. To create constitutive equations that are rotationally invariant all that is needed now is to formulate them in reference coordinates. For this purpose, we employ the standard rotationally invariant measures of strain and electric field [2,3]. To develop expressions for the (Piola-Kirchoff) stress tensor and polarization vector in terms of S_{KL} , W_L , n , and T , and for φ_n on n and T , we base them on an electric Gibbs free energy function Ψ and an electron function ε^n with the former expression including elastic and electric terms to third order [4]. The equations that result are:

$$\begin{aligned} \tau_A = & \tau_A^0 + C_{AB}[S_A - \alpha_A(T - T_0)] - e_{KA}W_K \\ & - \frac{1}{2}b_{AMN}W_MW_N - k_{KAB}W_KS_B + C_{ABC}S_AS_B \end{aligned} \quad (3a)$$

$$\begin{aligned} P_K = & P_K^0 - \lambda_K T + \chi_{KL}W_L + e_{KA}S_A \\ & + b_{KLA}W_LS_A + \chi_{KLM}W_LW_M + \frac{1}{2}k_{KAB}S_AS_B \end{aligned} \quad (3b)$$

where the indices A , B , and C range from 1 to 6 according to the usual shorthand, the dependence on the electron density is that for the electron gas equation of state when Maxwell-Boltzmann statistics are appropriate, and the last four terms are the additional constitutive nonlinearities considered in this paper. The material constants C_{AB} , C_{ABC} , χ_{KL} , χ_{KLM} , c_p , e_{KA} , k_{KAB} , b_{KLA} , α_B , and λ_K are the second- and third-order elastic, second- and third-order electric susceptibility, specific heat, piezoelectric, first odd electroelastic, electrostrictive, thermal expansion, and pyroelectric coefficients, respectively. The quantities τ_{KL}^0 and P_K^0 are the intrinsic stress and spontaneous polarization, respectively, and T_0 is a reference temperature. To make use of (3a) and (3b) in (1) it is necessary to transform them back to present coordinates using (3). Also note that (3a) and (3b) differ from expressions used previously in two respects that can become important when the displacements are not small. The first is associated with the nonlinear strain and electric field, and are referred to as kinematic nonlinearities. And the second enters through the last three terms in (3a) and (3b) and are known as constitutive nonlinearities. The particular effects included in (3) are called third-order electric susceptibility (χ_{KLM}), electrostriction (b_{AB}), electroelastic effect (k_{KAB}), and third-order elasticity (C_{ABC}), and some coefficient values as estimated from density functional theory [5]. All else is taken to be as discussed in [1], including the remaining con-

stitutive equations and values for their coefficients. The additional terms needed for time-dependent problems are also much like those presented in [1].

A final element of the theory is the boundary conditions, and these are treated as in [1] except for the conditions where the solid materials abut air/vacuum since the fundamental mapping in (2) is not defined in the latter [4]. In effect, this represents a third type of nonlinear correction in the theory. An elegant method for handling this aspect is the ALE (Arbitrary Lagrangian-Eulerian) technique [6] wherein the electrostatics in the air/vacuum region is solved for with the interface position being determined as part of the solution. To solve boundary value problems within the nonlinear theory we use the finite-element method as implemented in the powerful COMSOL package [7]. Especially convenient for our work is that this package offers the ALE method as an option.

III. SIMULATION RESULTS

To illustrate the finite deformation theory of this paper and to assess the importance of its nonlinearities, we consider several GaN device situations, all modeled in 2-D using a plane strain approximation with the epitaxial strain in the third direction incorporated analytically as in [1]. Also for purposes of efficiency, as in [1] we embed the electrically active region in a larger thermomechanical structure.

The first example is a conventional GaN HEMT with a 25nm $Al_{0.3}Ga_{0.7}N$ barrier that was studied extensively in [1] using linear theory. In Fig. 1 we compare simulated I_D - V_G and I_D - V_D characteristics obtained using the full nonlinear theory with those obtained from linear theory. The nonlinear corrections are found to be small ($<10\%$) but with non-negligible electrical consequences with $\Delta V_T \sim 0.2V$ and $\Delta I_{max} \sim 5\%$. Further simulations reveal that the electrical corrections are largely constitutive in origin and derive mainly from the nonlinear polarization. Not surprisingly an analogous device that had a 10nm AlN barrier showed a larger nonlinear correction with $\Delta V_T \sim 0.4V$.

We next consider the stress concentrating effect of a small crack in the AlGaN barrier of the device as was studied previously using linear theory [1]. As shown in Fig. 2, under high-power conditions ($V_G = 0V$, $V_D = 20V$) the tensile stress at the crack tip is calculated using the nonlinear theory to be 13GPa which is 1.1GPa smaller than that estimated using linear theory [1]. From the nonlinear simulation we also find the device to be displaced upward by about 7nm as a result of thermal expansion.

The next example is a “GaN-on-Air” HEMT concept in which cooling is provided by a CVD nanocrystalline diamond over-coating [8]. Fig. 3 compares the drain characteristics for this device as computed by the linear and nonlinear theories. The temperature field and heat flux streamlines are shown in Fig. 4. With a 0.5 μm thick layer of NCD, the peak temperature is elevated by only about 40°C over a conventional HEMT when $V_D = 10V$.

As a final example, we simulate an AlGaN/GaN MEMS cantilever operating as a nanogenerator [9]. This device harvests mechanical kinetic energy by converting it into electrical

energy. Fig. 5 shows solution profiles for the electric potential, electron density, and on-axis stress that exist in the cantilever when under mechanical load. The potential derives largely from piezoelectrically generated charge that in turn enhances or depletes mobile charge from the GaN as illustrated for a different device geometry in Fig. 76; this figure also shows the range of validity of linear simulation. When driven by a sinusoidal load, these charge variations translate into an ac current. It should be noted that because of the particular cantilever design and the size of the mechanical load, maximum tensile stresses can rise as high as 10GPa and may well exceed the tensile strength of the materials [1].

IV. FINAL REMARKS

The equations of the nonlinear thermoelectromechanical theory of piezoelectric semiconductors are presented and discussed. The theory is then illustrated with applications to several GaN device situations with emphasis on its departures from linear theory and their origins. In general, the nonlinear theory is apropos when the mechanical strains and/or the mechanical rotations are large.

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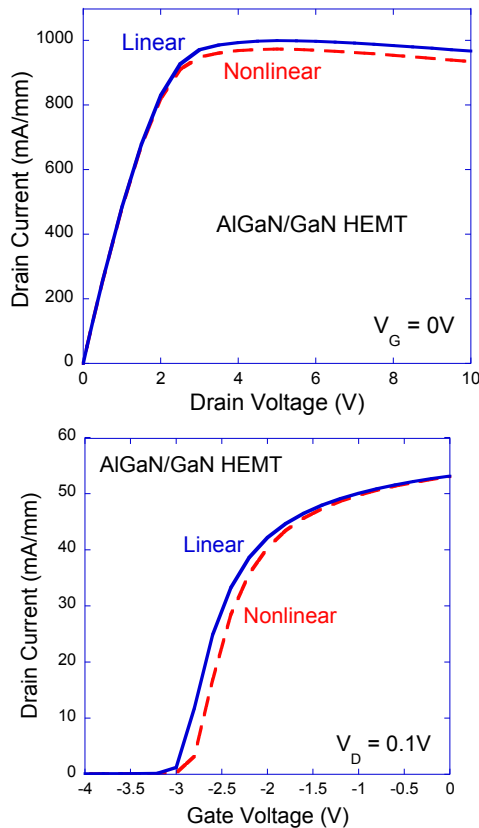


Fig. 1. Simulated (a) drain and (b) transfer characteristics for an AlGaIn/GaN HEMT and comparing linear and nonlinear theory.

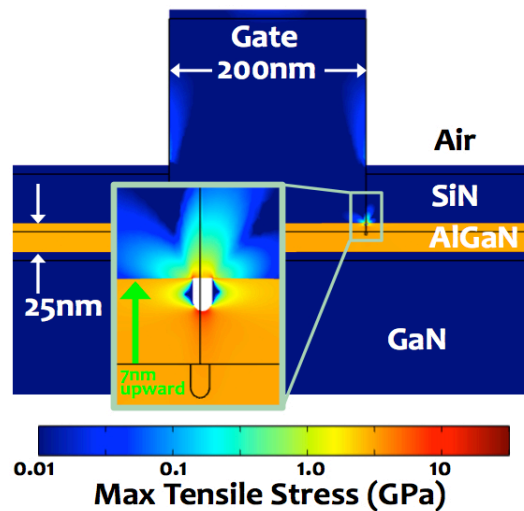


Fig. 2. Stress in a AlGaIn/GaN HEMT with a crack at the drain edge of the gate. Nonlinear correction to the maximum is about 1GPa. Note upward displacement due to thermal expansion.

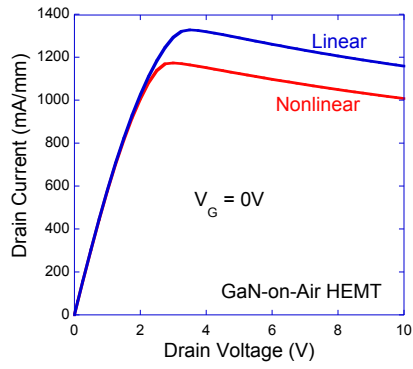


Fig. 3. I-Vs of the GaN-on-Air device comparing linear and nonlinear simulations.

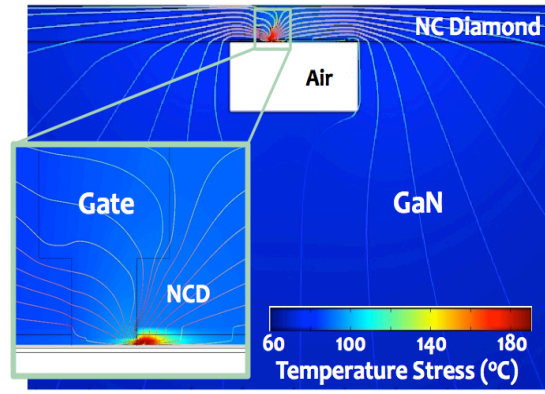


Fig. 4. Temperature distribution and heat flux streamlines in the GaN-on-Air device with $V_D = 10V$.

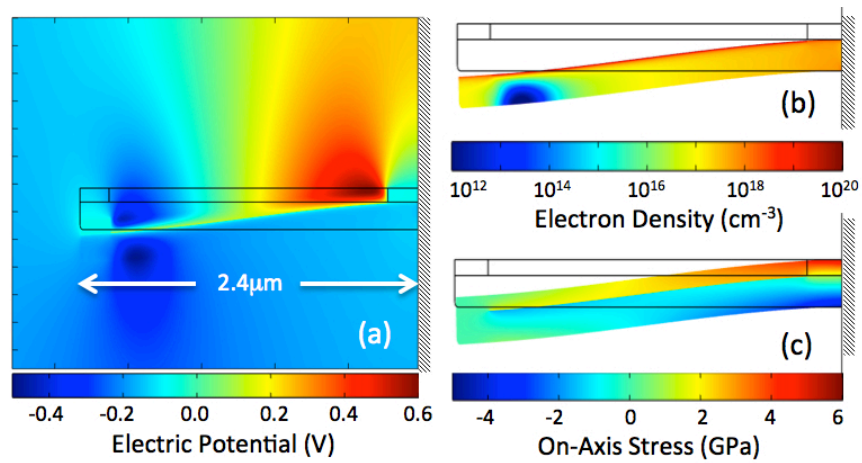


Fig. 5. Solution profiles for (a) electric potential, (b) electron density, and (c) on-axis stress for an AlGaIn/GaN nanogenerator with force applied to the left end.

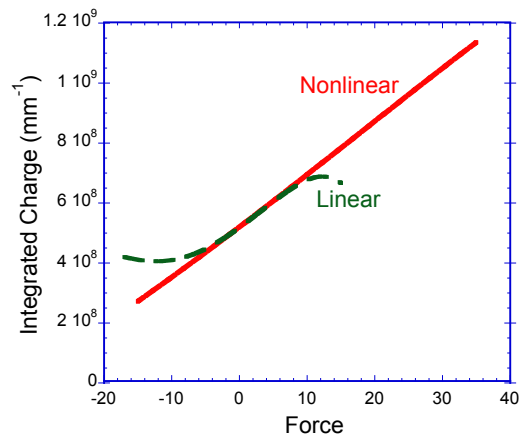


Fig. 6. Stored charge vs applied force on a nanogenerator and comparing linear and non-linear results.