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Thermoelectromechanical Simulation of GaN HEMTs

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***Abstract*—As a tool for studying the critical issue of reliability in GaN HEMTs we develop a multi-dimensional device simulator based on a continuum formulation in which the electrical, mechanical, thermal and transport variables are fully coupled. The new simulator is illustrated with various examples involving HEMT operstion and failure.**

Keywords-GaN HEMTs; reliability; failure mechanisms; multi-dimensional simulation; thermoelectroelastic; piezoelectric; thermal expansion; diffusion-drift.

I. INTRODUCTION

The basic quantitative understanding of the role and importance of spontaneous and piezoelectric polarizations in GaN HEMTs was established in the papers of Ambacher *et al.* [1]. Through careful experiments and 1-D calculations they showed how the dipole nature of GaN, AlN and their alloys produces polarization charges that, in appropriate device structures, induce very high mobile charge densities. Knowledge of this physics and of the relevant material constants led to much further research as well as to practical applications, including an interest in N-face devices and the use of indium alloys as a means of combatting excessve strain. With respect to reliability, an intriguing proposal was that from del Alamo [2] and Chowdhury [3] suggesting that piezoelectric strains in biased HEMTs could be the triggering mechanism for the degradation observed in these devices. All of this progress in understanding GaN HEMTs also led to significant work in device modeling [4-6], however, a full treatment with "all" of the electrical, mechancal, thermal and transport variables included in a fully coupled manner and in multi-dimensions has not been given heretofore. This is the goal of the present contribution with our prime interest being in developing a tool for understanding GaN HEMT failure physics and for creating device designs with improved reliability.

II. GOVERNING EQUATIONS

A. Modeling Approach

While trying to use physics-based modeling to aid the understanding of GaN HEMT reliability is certainly a worthy goal, it should also be recognized that it is a challenging one. The difficulty comes largely from the need to understand devices in the extreme circumstance of being pushed to failure. This usually brings in many different phenomena and generally drives the models well beyond their range of applicability. Also, experiment — and especially the post-mortem examination of a failed device — rarely provides an unambiguous view of what one really wants to know, namely, the factor(s) that triggered the failure. In particular, experiments on stressed GaN HEMTs show that the electrical degradation is accompanied by increased trap density, increased gate current, and physical pits/cracks in the AlGaN barrier layer, typically at the gate's drain-side corner (see Fig. 1). However, what is causal in this complex situation is hardly clear, and so one looks to further experiment and/or to modeling for help.

Given the complexities of electron trap generation and the mechanical failure of materials, a full physics-based model of GaN HEMT failure is presently impossible. Nevertheless, many aspects of the problem can be modeled and one can learn much about the electrical, mechanical, and thermal conditions that prevail inside the device under accelerated life-testing conditions. Although microscopic approaches based on the Boltzmann equation can be useful [7], we employ here a more conventional continuum approach. The device structure modeled in this paper is the standard GaN/AlGaN HEMT design as used in RF and power electronics, and as depicted in Fig. 2.

B. Equations

The thermelectromechanical model for AlGaN/GaN HEMTs developed in this paper consists of the fully coupled equations of electroelasticity, diffusion-drift transport, and linear heat conduction with steady-state conditions assumed. This means that inside the GaN the governing PDEs are:

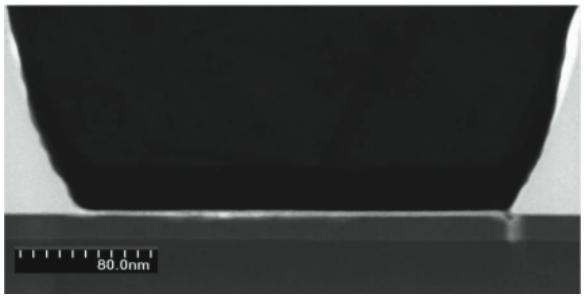

Figure 1. TEM X-section of a failed GaN HEMT from [3].

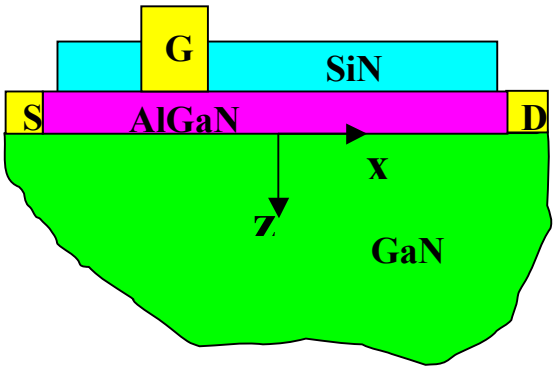

Figure 2. GaN HEMT device structure.

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$$\nabla\cdot\mathbf{D}=q(N-n) \qquad \nabla\cdot\mathbf{J}=0 \qquad \mathbf{J}=qn\mu_n\nabla(\varphi_n-\psi) \qquad (1a)$$

$$\nabla\cdot\tau=0 \qquad \nabla\cdot\mathbf{q}=\mathbf{J}\cdot\nabla(\varphi_n-\psi) \qquad (1b)$$

where N is a possible bulk charge density (due to ionized impurities or fixed charge), the right side of $(1a)_2$ being zero means we neglect electron generation-recombination effects, and the right side of the last equation in $(1b)_2$ gives the Joule heating associated with the diffusion-drift transport in the GaN (with no contribution from recombination). The quantities **D** and τ are the electric displacement vector and the mechanical stress tensor, respectively, for which we assume the ordinary linear electroelastic constitutive equations including terms representing the spontaneous polarization, the intrinsic stress, and thermal expansion. The vector **q** is the heat flux that we assume to obey the Fourier law. All other variables and parameters have their usual meanings, and we assume the values for the material constants are as given in [1]. Obviously in electrical insulators and in metals not all of the equations in (1) apply.

Because GaN HEMT devices are typically far wider than they are long, it is appropriate to consider a 2-D plane-strain treatment of their electromechanics. In principle, however, such an approach is invalidated by the epitaxial growth which introduces a 3-D strain field consisting of the biaxial in-plane deformation imposed by the growth plus an out-of-plane strain resulting from Poisson's ratio. But since the in-plane epitaxial strain is set by the thick GaN buffer and the known composition of the overlayers, it can be subtracted out analytically leaving the remainder of the problem to be solved numerically in 2-D. This is the procedure employed in this paper.

In addition to the PDEs one must of course also have BCs which are standard with three exceptions. First, at free surfaces it is generally the case that the polarization charge will be neutralized by adventitious charges, and these must be introduced into the calculation explicitly. Second, we include contact resistance chosen so that the drain current in the ON-state is roughly 1A/mm as it is in high-quality GaN/AlGaN HEMTs. And finally, we include a thermal resistance BC to represent the unsimulated bulk thickness of the substrate as well as the packaging, and calibrate it with thermal results obtained on state-of-the-art GaN HEMTs by one of our industrial partners.

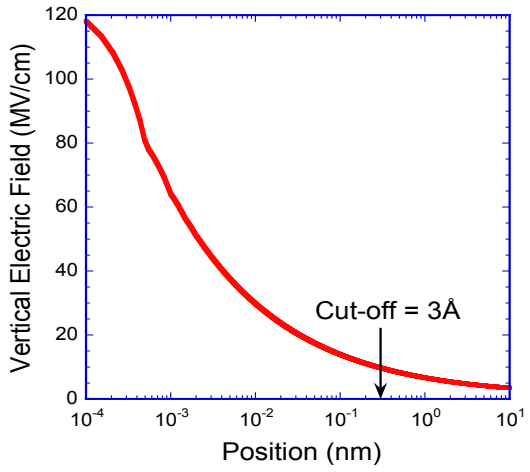

Figure 3. Electrc field calculated in close proximty to the gate corner and showing singular behavior.

C. *Singular Solutions*

Just as in elasticity and electrostatics, when corners/cracks are treated as mathematically sharp (i.e., with vanishing radius of curvature), the solutions to the equations of Section IIB will often develop singularities. These spurious infinities originate from the continuum theory ignoring the material's underlying lattice structure. A rigorous analysis of the situation would require joining a "far field" continuum solution to a microscopic representation of the "core" region of the corner/crack. However, lacking knowledge of the precise geometry, such an elaborate treatment seems pointless, and so instead we ignore the microscopics entirely and simply truncate the continuum solutions with a cut-off distance. As illustration, for a GaN HEMT structure like that of Fig. 2, in Fig. 3 we plot the electric field profile along the gate/AlGaN interface as a function of distance from the drain corner. The field maximum as computed numerically grows without bound as the mesh is refined, appearing to become singular as $1/x^{1/3}$. The rapid increase is clearly confined to within ~1Å of the corner, and it is in this regon that the continuum treatment is clearly invalid. Based on the plot in Fig. 3, in this work we assume a cut-off distance of 3Å (i.e., roughly the size of the unit cell).

D. *Failure Criteria*

While the continuum treatment does capture many key aspects of the GaN HEMT physics, as noted above it also omits much that is critical including trap generation and mechanical failure. Our approach to dealing with such degradation is to employ certain metrics to judge when and where failure may be triggered. Specifically, we take the primary electrical factor influencing degradation/failure to be electron injection into the AlGaN barrier, and so use as our *electrical metric* the threshold electric field at which significant Fowler-Nordheim injection can be expected. Given a Schottky barrier height of 1.35eV [8] and a tunneling distance of ~2nm, the threshold electric field will be ~9MV/cm. The mechanical factor that we assume crucial to inducing degradation/failure is excessive tensile stress, and so use as a *mechanical metric* the size of the stress as compared to AlGaN's tensile strength. Theoretical estimates of AlGaN's tensile strength are not reliable, but it is worth noting that the energy required to create two AlGaN surfaces (to form the faces of a crack) is ~2 x 0.12eV/Å^2 [9], and with a lattice constant of about 3Å, this imples an energy density to produce the break of ~80meV/Å^3 or 13GPa. More concretely, in Fig. 4 we plot the in-plane stresses and strains generated in $Al_xGa_{1-x}N$ /GaN heterostructures. That epitaxial AlN layers of a few nanometers can be successfully grown on GaN suggests a similar yield strength of ~10GPa. But beyond this it seems impossible to say how tough the AlGaN in the vicinity of the gate corners of a HEMT might actually be given our lack of knowledge of the precise geometry as well as the likelihood of synergistic effects, e.g., defects or Joule heating weakening the material and making mechanical failure more likely.

E. *Verification*

Although the theory of Section IIB is the accepted continuum description of the electromechanics of GaN/AlGaN heterostrucures, the evidence for its validity is not as strong as one would like. One source of error could easily be inaccuracy in some of the material constants for the ultra-thin layers of interest. More fundamentally it may be that the use of linear theory is itself in question when the strains are as large as they are in the AlGaN. In any event, in this paper we ignore all such issues and limit our "verification" to demonstrating good agreement between our numerical simulations and results for 1-D heterostructures that have been reported in the literature. The specific comparison is for a heterostructure consisting of a GaN substrate and an epitaxial $Al_xGa_{1-x}N$ overlayer, and we compare 1-D analytical results from [1] for the piezoelectric charge and the total polarization charge at the AlGaN/GaN interface with results obtained by solving the equations of Section IIB numerically. The agreement (not shown) is excellent.

III. Results and Discussion

To illustrate the thermoelectromechancal simulator, we apply it to simulating the GaN HEMT of Fig. 2 with a 25nm barrier of $Al_{0.3}Ga_{0.7}N$, a 50nm passivating layer of SiN, a gate length of 0.3μm, a gate-to-drain spacing of 1.6μm, and with the gate placed closer to the source contact as shown in the figure. To set a baseline, in Fig. 5 we show the calculated drain characteristics in which I_{DSS} takes the realistic value of ~1A/mm (as a result of our choice for the contact resistance as noted earlier). In the ON-state, we find the maximum electric field is ~5.8MV/cm, the maximum principal stress is ~3.5GPa, the maximum strain is ~0.75%, and the maximum temperature is ~129C, with all of these values occurring in the AlGaN at the drain-side corner of the gate. While these values are of significant size, in conformity with experiment they seem not so large as to lead to "rapid" device failure in the ON-state.

A. *Effect of bias-stress.*

Accelerated life testing is often employed to evaluate device reliability. In this paper we focus on a "high-power" stressing condition with V_{GS} = 0V and V_{DS} = 20V under which the maximum power dissipated is about 15W/mm. The simulated maximum channel temperature is around 400C, a temperature that may be sufficient to itself cause device degradation by activating "chemical" processes such as the surface diffusion of atoms. To better understand the thermoelectromechanical fields under high-power conditions we next examine in Fig. 6 1-D cutline profiles across the AlGaN at the drain corner of the gate of the electron energy, the electric field, the maximum principal stress and the piezoelectric contribution to the stress. The peak electric field is ~11.5MV/cm at the gate edge and, as the Figure indicates, this produces a barrier less than 2nm wide, and we expect strong electron injection. The maximum stress is ~4.6GPa, of which roughly 0.5GPa is piezoelectric and 0.6GPa is thermal in origin. That the thermal contribution is as large as the piezoelectric argues against the latter being decisive. But in any case the total stress, though elevated over that in the ON-state, still seems insufficient to trigger pit/crack formation directly, unless the very high operating temperature and/or the strong electron injection act to lower the threshold for material failure.

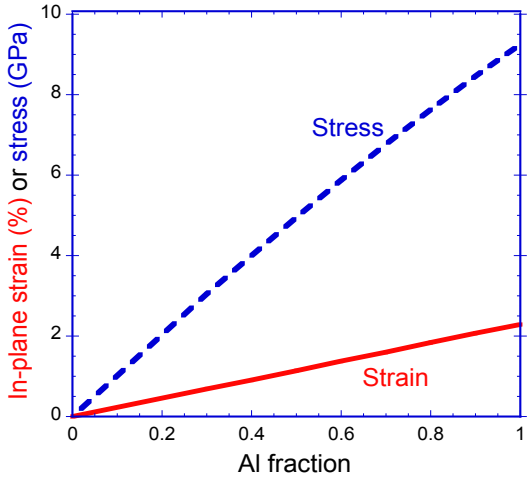

Figure 4. Stresses and strains in 1-D AlGaN/GaN heterostructures.

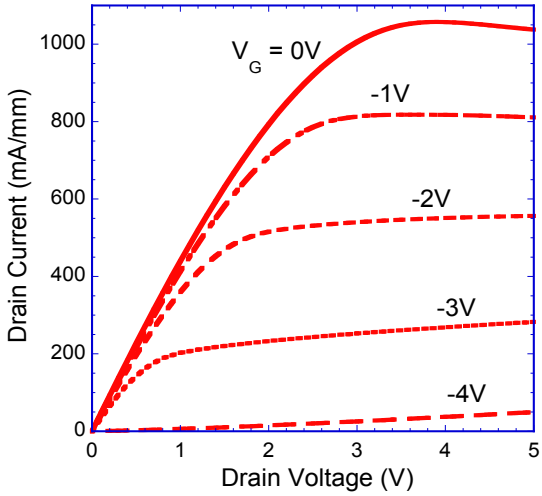

Figure 5. Simulated drain characteristics of the GaN HEMT.

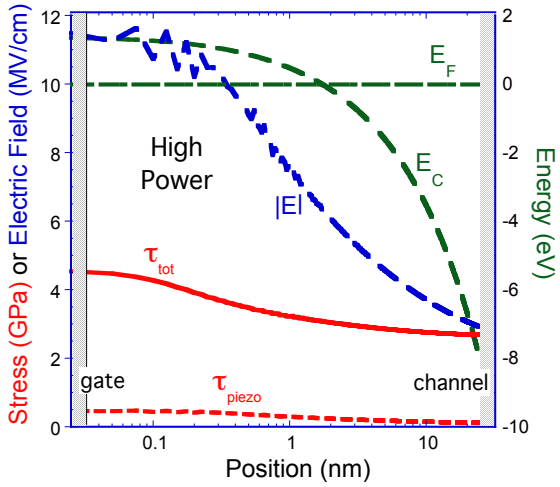

Figure 6. Solution profles across the AlGaN layer under high-power stressing condtions.

B. *Fracture*

When sufficiently stressed, the AlGaN will undergo brittle fracture via two sequential steps, crack initiation followed by crack propagation. Of the two, judging whether and how crack initiation takes place is far more complicated for many reasons already discussed. But whatever the cause, it is an experimental fact that stressing under high-power conditions often results in the formation of pits and/or incipient cracks in the AlGaN barrier layer [3]. Our approach to crack propagaton is to compare the maximum principal stress developed at the crack tip with the tensile strength of the material with the idea that propagation will occur so long as the stresses at the tip are high enough to cause continued rupture of the lattice. A sample result of a "damaged" GaN HEMT in which a 2x3nm "pit" has been introduced at the drain-side corner of the gate is shown in Fig. 7. We observe that the peak stress is now much higher (13GPa versus 4.6GPa) than it was with no crack present. The increase in stress is due to the concentrating effect of the "groove" and will be reduced if the radus of curvature of the initiating crack is made larger. Based on our earlier discussion, this level of stress is likely above the tensile strength of the AlGaN, and so our analysis indicates that this very small crack will propagate. And as the crack deepens, the stress is found to continue to rise (to 35GPa when the crack has almost fully travserved the AlGaN layer) implying that the crack will continue to propagate, and will quickly traverse the AlGaN layer as is seen experimentally, e.g., as in Fig. 1 [3]

As noted earlier, a crucial issue regarding GaN HEMT failure is causality. For example, do the pits/cracks *cause* the device's electrical degradation or do they merely accompany a separate electrical damage pathway. One aspect of this causality issue that is readily explored with simulation is to ask to what extent the existence of the crack itself affects the device I-V characteristics. The simulated I-V curves appear in Fig. 8 where we compare the devices with no damage, with a small crack as in Fig. 7, and with a crack that extends nearly across the AlGaN layer. Clearly the small crack has little effect on the current whereas the large crack has a substantial impact. This electrical degradation is produced by the polarization fields generated around the large crack that induce an electrostatic barrier in the channel, thereby impeding the current.

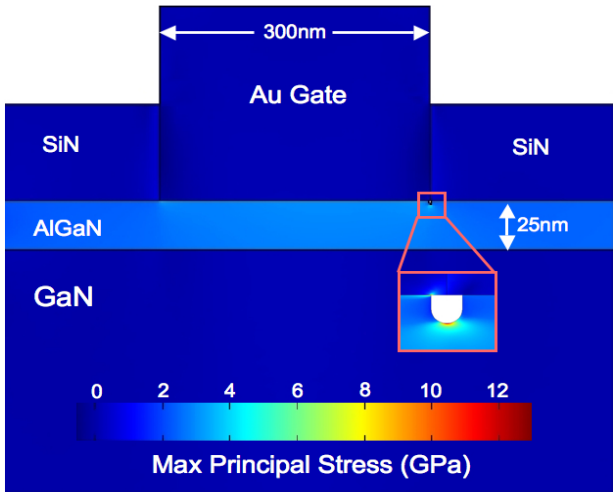

Figure 7. Simulated maximum princple stress in a "damaged" GaN HEMT showing the large increase in stress induced by the "crack".

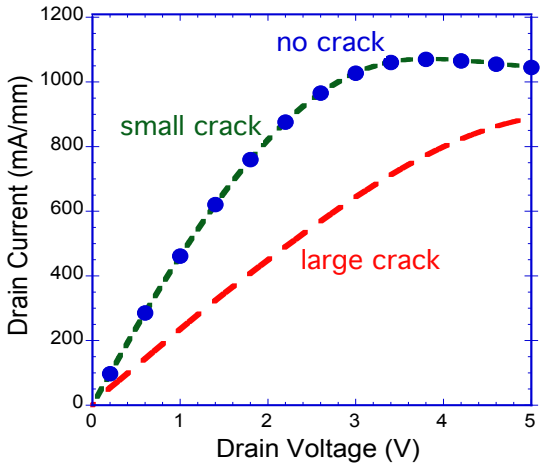

Figure 8. Simulated I-V curves of GaN FETs wth no crack, a small crack, and a large crack nearly traversing the AlGaN.

IV. Final Remarks

A tool has been introduced for performng fully coupled, mult-dimensional analysis of the thermoelectromechancs of GaN HEMTs. As llustrated herein, we expect the simulator to be useful for improving the performance and reliabilty of nitride devices in rf and power electronics applications.

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