A Self-Consistent Electro-Thermo-Mechanical Device Simulator based on the Finite-Element Method

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Abstract—**The Florida Object-Oriented Device Simulator (FLOODS) has been augmented to perform self-consistent, electro-thermo-mechanical simulations. We show simulation examples of a MEMS thermal actuator and an AlGaN/GaN HEMT in good agreement with commercial tools and literature. An example of a degradation mechanism in an AlGaN/GaN HEMT is also presented. FLOODS uses finite-element discretization methods to provide the first fully-coupled solver in all three domains.**

Keywords-device simulation; electro-thermo-mechanical simulation; finite-element method; AlGaN/GaN HEMT degradation

I. INTRODUCTION

Multiphysics modeling is useful for a variety of applications. The modeling of some micro-electro-mechanical systems (MEMS) requires physics from the electrical, thermal, and mechanical domains. Thermal actuators, for example, rely on Joule heating of materials that have mismatched coefficients of thermal expansion to induce mechanical deformation. Similarly, electro-thermo-mechanical (ETM) simulations enhance reliability assessment and performance prediction of AlGaN/GaN high electron mobility transistors (HEMTs). Under normal operating conditions these high-power devices can undergo significant self-heating and non-uniform strains may arise due to the inverse piezoelectric effect in the AlGaN and GaN layers.

Multiple commercial tools handle various aspects of multiphysics modeling and tend to be application specific. Silvaco Atlas and Sentauraus SDevice are routinely used for modeling transistor device performance since their handling of electronic transport in semiconductors is robust. They each have fully coupled, electro-thermal solvers, but limitations in the mechanical domain. Atlas does not have a mechanical solver and SDevice does not support the inverse piezoelectric strain or a temperature dependence on Young's modulus. COMSOL provides ETM simulations and is well suited for MEMS among many other modeling applications where electronic transport in semiconductors is unnecessary.

Up to now, researchers who need to model in all three domains and a rigorous treatment of electronic properties in semiconductors use a combination of commercial software packages or write their own code. Venkatachalam et al. used a combination of Sentaurus for the electrical simulation and COMSOL for the thermal-mechanical simulation to model GaN-based HFETS [1]. Gao et al. used Silvaco Atlas and in-house software to simulate ETM effects on a GaN HEMT [2]. In both cases the mechanics were one-way coupled to the electrical part. Thus, any strain-induced change on electrical performance could not be captured. One group has amassed capability of fully-coupled simulation of strain and electronic transport in nanostructured devices [3]. However, thermal effects were not considered.

Fully-coupled ETM simulations could benefit reliability assessment of AlGaN/GaN HEMTs. Horton et al. show that mechanical strain in the device enhances impurity diffusion on the drain side of the gate in the off state, which ultimately affects I-V characteristics [4].

We have augmented the Florida Object-Oriented Device Simulator (FLOODS) to handle physics in the electrical, thermal, and mechanical domains in a fully coupled, self-consistent way using the finite-element discretization method (FEM). This solver is both general and specific enough to support many different applications (eg. MEMS and semiconductors devices) and is flexible enough to account for new physics in a simple way. The structure of this paper is as follows: the general differential equations used to comprise the ETM domains are discussed along with our approach to numerical discretization in Section II. Section III includes comparisons of simulation results to commercial software and a novel application of ETM modeling on an AlGaN/GaN HEMT.

II. ETM PHYSICS AND SIMULATION METHODS

The common partial differential equations that model electrostatics and charge transport in semiconductors, heat conduction, and linear elastic behavior of solids are presented in (1-5).

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$$\nabla^2\psi = -\frac{q}{\varepsilon_p}(p - n + N_D - N_A) \quad (1)$$

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla\cdot J_n - r_n + g_n \quad (2)$$

$$\frac{\partial p}{\partial t} = \frac{1}{q}\nabla\cdot J_p - r_p + g_p \quad (3)$$

$$c\frac{\partial T}{\partial t} - \nabla\cdot K\nabla T = Q \quad (4)$$

$$\nabla\cdot\sigma = 0 \quad (5)$$

The Poisson equation is given in (1), where ψ is electrostatic potential, n is the density of electrons, p is the hole density, N_A and N_D are ionized acceptor and donor densities, respectively, q is charge, and ε_p is permittivity. Equations for continuity of electrons and holes are given in (2-3), where J_n and J_p are the electron and hole current densities, respectively, and r and g are recombination and generation terms. The thermal domain is characterized by the heat conduction equation (4), where T is temperature, c is the specific heat capacity, K is thermal conductivity, and Q is the heat generation term. The mechanical equilibrium equation (5) governs elastic deformation with no external forces. Stress σ is related to strain ε by the constitutive relation $\sigma=D(\varepsilon-\varepsilon_0)$, where D the stiffness matrix is a function of Young's modulus and Poisson's ratio. Mechanical strain caused by a mismatch of the thermal coefficient of expansion between two materials is modeled by a definition for initial stress given as

$$\varepsilon_0 = \alpha_{mismatch}\Delta T, \quad (6)$$

where $\alpha_{mismatch}$ is the difference in the coefficients of thermal expansion. Strain due to the inverse piezoelectric effect is modeled by (7)

$$\varepsilon_0 = \nabla\psi\cdot d_{pz}, \quad (7)$$

where d_{pz} is the matrix of inverse piezoelectric coefficients.

The Scharfetter-Gummel (SG) formula and finite volume or finite-difference discretization schemes have historically made mathematical modeling of electronic transport in semiconductors possible. In this method, the formulation of the current density, J_n and J_p, in the continuity equations includes separate drift and diffusion terms. Many commercial and noncommercial device simulators including PICES-II, PADRE, Sentaurus SDevice, and Silvaco Atlas are based on this method. On the other hand, mechanical solvers conventionally employ finite-element methods. Solving coupled, partial differential equations in the three domains in a concurrent and self-consistent way poses a computational challenge if different discretization methods are used. We have circumvented this challenge by formulating the drift and diffusion current as quasi-linear functions of the gradients of the quasi-Fermi levels and using finite-element methods to disctretize the electron and hole continuity equations. An example of this formulation for electron current density is given below

$$J_n = -q\mu_n n\nabla\phi_n, \quad (8)$$

where μ_n is mobility and ϕ_n is the quasi-Fermi level that can be related to the electrostatic potential by the Boltzmann relation. A previous paper shows good agreement between a finite-volume method based on the Scharfetter-Gummel formula and the afore-mentioned finite-element method based on the quasi-Fermi representation; plus the FEM approach showed even better numerical accuracy for applications that require isotropic current flow [5]. With this method, a heat generation term due to Joule heating may be directly computed using the formulation given in (9) [6].

$$Q = q\,|J_n|^2/(\mu_n n) + q\,|J_p|^2/(\mu_p n) \quad (9)$$

III. Simulation Results

A. Calibration

To validate FLOODS' ETM capabilities, 2-D simulation results from FLOODS are provided on examples of a MEMS thermal actuator and an AlGaN/GaN HEMT and compared to results from COMSOL or Sentaurus. The first results are for a thermal actuator. Fig. 1 shows the mechanical deformation caused by a 3 V bias on the resistive heating element inside the bimorph beam. Dirchlet boundary conditions for the displacement and temperature were assigned to the bottom of the structure (bulk Si). Small deformation and plane strain approximations were used for both simulations. Fig. 2 shows good agreement between results from FLOODS and COMSOL of displacement along the top of the beam.

Next, an electro-thermal simulation of an AlGaN/GaN HEMT in FLOODS is compared to one done in Sentaurus SDevice. The HEMT structure used in both simulators consisted of an undoped 1.0 µm SiC substrate, an undoped 0.20 µm AlN layer, a 1.775 µm GaN layer with an acceptor doping level of 6.5e16 cm^{-3}, and an undoped 0.025 µm

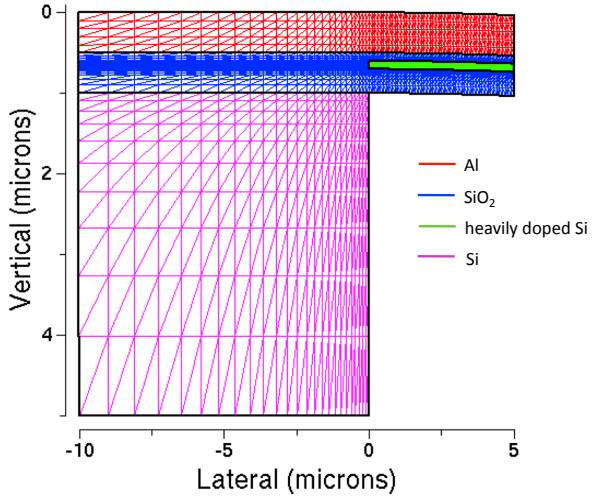

Figure 1. FLOODS electro-thermo-mechanical simulation of a 2-D MEMS thermal actuator showing the resulting beam deformation with 3V bias across the polySilicon heater.

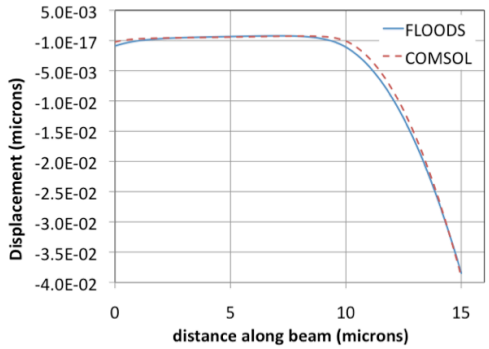

Figure 2 – Electro-thermo-mechanical simulation validation on a 2-D MEMS thermal actuator showing vertical displacement at the top of the beam. The FLOODS results are compared to COMSOL results.

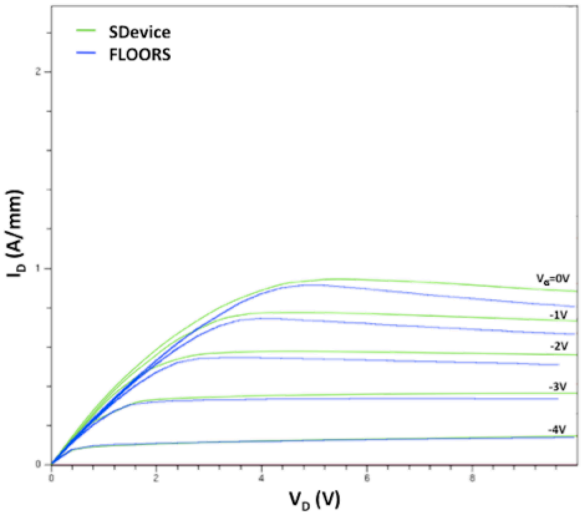

Figure 3. Drain current as a function drain voltage for various gate voltages of an AlGaN/GaN HEMT. The FlOODS simulation results are compared to results from Sentaurus SDevice.

$Al_{0.26}Ga_{0.74}N$ layer. The structure was 4.0 µm wide. A 0.25 µm t-gate was contacted at the center of the surface of the AlGaN layer and source and drain were contacted to the AlGaN at the left and rightmost regions of the layer. An insulating oxide layer was created on top of the AlGaN layer that also surrounded the contacts. An interface charge of 1.17e13 was placed between the AlGaN and GaN layers to reflect the spontaneous and piezoelectric polarization charge. Fig. 3 compares I-V plots for gate voltages ranging from 0 to -4 V. The characteristic decrease in drain current from self-heating at high drain bias is in good agreement with theory. The main difference in the curves is due to the treatment of the heat generation term. The influence of the inverse piezoelectric effect and self-heating can be seen in the plot of vertical strain right below the AlGaN surface shown in Fig. 4. The compressive strain peaks at the drain edge of the gate due to a corresponding peak in electric field and is in good qualitative

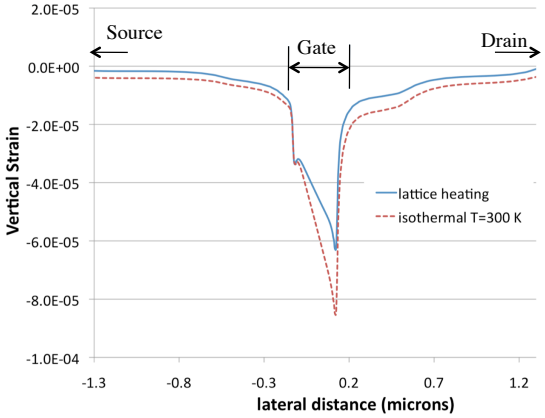

Figure 4. Effect of lattice temperature on the vertical strain along the AlGaN layer of a HEMT simulated in FLOODS. The ETM model shows a decrease in compressive strain from the isothermal case, relating relaxation of the lattice. The bias conditions are Vgs=0.0 V and Vds=3.0 V.

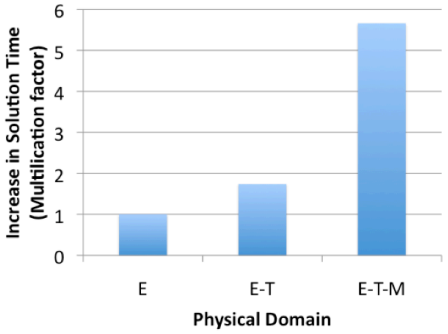

Figure 5. Comparison of solution time for the electrical-only, electro-thermal, and electro-thermo-mechanical simulations in FLOODS.

agreement with simulation results from Gao et al. [2]. For the HEMT simulation, the Youngs's modulus was made dependent on temperature. Thus at elevated lattice temperatures, the decreased Young's modulus and addition of tensile strain due to thermal expansion of the AlGaN act to decrease the compressive strain as compared to an isothermal simulation shown in Fig. 4.

Fig. 5 compares the increase in simulation time with increase in domains. Electro-thermal simulations take about twice as long to run than electrical simulations, while electro-thermo-mechanical simulations take about six times as long as electrical simulations.

B. Example: Reliability Study of an AlGaN/GaN HEMT

The following example shows the versatility of FLOODS in an AlGaN/GaN HEMT reliability study. To capture the physics of defect formation and electrical degradation of the HEMT as seen in step-stress experiments, we performed a multistep simulation. First an electro-mechanical simulation was performed to generate strain profiles at various electrical stresses. Fig. 6 shows the resultant strain contours within the device when in the "off" state with Vg = -5V and Vdg = 40V.

(A coupled thermodynamic simulation was not needed since there is minimal Joule heating in the "off" state.) This spatially varying strain produced from the electro-mechanical simulation was then used as the input to a strain dependent diffusion model also simulated in FLOODS. Here the gate metal was allowed to diffuse into the AlGaN layer with a strain-altered diffusivity [4]. A typical simulation result is compared to a TEM image of the gate area in a degraded HEMT in Fig. 7. The generated diffusion profile matches quite well with observed metal diffusion reported by Holzworth et al. [7]. Implementing a number of diffusion profiles in Poisson's equation as additional dopants generated the resulting I-V curves shown in Fig. 8. The self-heating effect is also taken into account via an electro-thermal simulation and can be seen in the characteristic decrease in Ids current at higher drain voltages in all cases.

These results indicate that future investigation of defect generation in AlGaN/GaN HEMTs in the "on" state would benefit from an ETM simulation coupled with impurity diffusion, all of which is capable in FLOODS.

I. Conclusion

We have augmented FLOODS to be capable of a fully-coupled ETM model using only the finite-element method. This is the first simulator capable of simultaneously solving partial differential equations in the electrical, thermal and mechanical domains, important for reliability and MEMS simulations.

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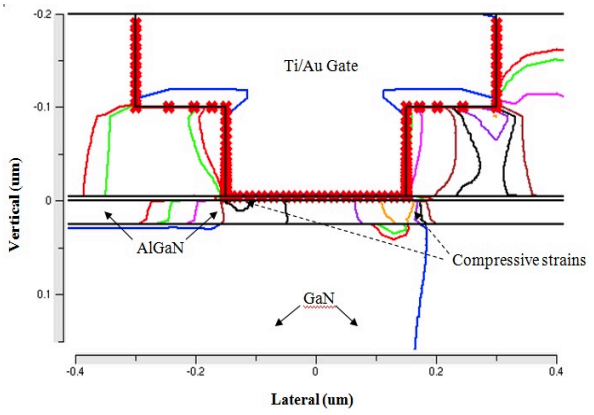

Figure 6. FLOODS electro-mechanical simulation of a GaN HEMT in the off-state. Mechanical strain contours due to the inverse piezo effect show highest vertical compressive strains of ~-7e-4 in the AlGaN layer at both edges under the gate, but much more pronounced on the drain edge (right side). Reprinted with permission from [4] ©2012 IEEE.

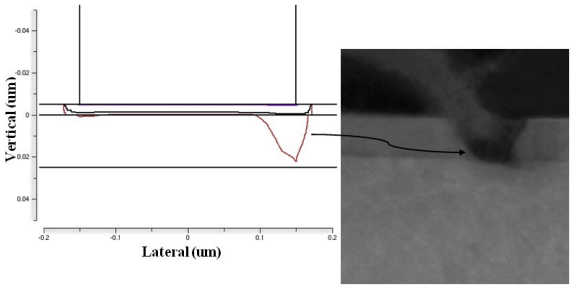

Figure 7. Simulation of metal diffusion compared to TEM close-up of gate area showing metal diffusion in the Off-state. Contours in simulation show enhanced diffusion at drain edge (right side) of gate where compressive strains are higher. Reprinted with permission from [4] ©2012 IEEE.

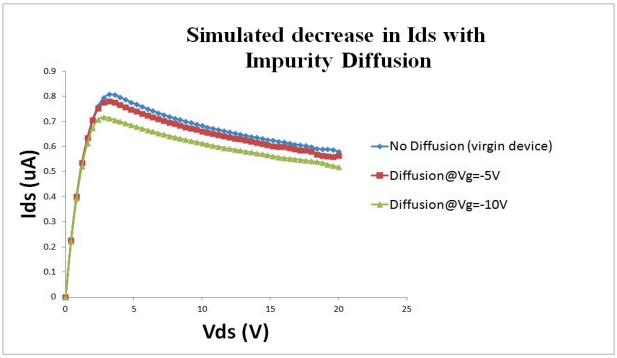

Figure 8. Simulated IV curves for increasing impurity concentrations. Top blue curve shows the simulated drain current for a device with no impurity diffusion into the AlGaN.

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