2001 International Conference on Indium Phosphide and Related Materials
Conference Proceedings
13th IPRM 14-18, May 2001 Nara, Japan

A Model for Hydrogen-Induced Piezoelectric Effect in InP HEMTs and GaAs PHEMTs

S. D. Mertens and J. A. del Alamo

Massachusetts Institute of Technology, Cambridge, MA 02139
smertens@mit.edu, alamo@mit.edu

Abstract

We have developed a model for the impact of the hydrogen-induced piezoelectric effect on the threshold voltage of InP HEMTs and GaAs PHEMTs. We have used 2D finite element simulations to calculate the mechanical stress caused by a gate that has exanded due to hydrogen-absorption. This has allowed us to map the piezo-electric charge distribution in the semiconductor heterostructure. We used a simple electrostatics model to calculate the impact of this piezo-electric polarization charge on the threshold voltage. We have found that the model explains experimentally observations of hydrogen-induced threshold voltage shifts, both in InP HEMTS and in GaAs PHEMTs.

I. Introduction

Hydrogen degradation has been identified as a serious reliability concern in III-V FETs in general and InP HEMTs in particular [1]. In applications demanding hermetically-sealed packaging, such as satellite or fiber-optic systems, exposure occurs when H out-gasses from the packaging material and becomes trapped inside the package cavity. Eventually H diffuses into the transistor and alters its electrical characteristics leading to parametric module failure.

Recent research has shown that H exposure results in the formation of TiH_x in Ti/Pt/Au gates [2]. This produces compressive stress in the gate, which generates a tensile stress in the heterostructure underneath. The resulting piezoelectric polarization charge causes a threshold voltage shift.

Literature reports of the sign and magnitude of the V_T shift in InP HEMTs and GaAs PHEMTs seem contradictory. While all reports on [011]-oriented GaAs PHEMTs show a positive V_T shift [3], [011]-oriented InP HEMTs have been found to display positive [4], negative [3], and even negligible V_T shifts [5]. When all the data are graphed together, however, a compelling picture emerges (Fig. 1). It appears that for GaAs PHEMTs, ΔV_T is always positive and increases as the gate length is reduced. However, no data exist for long devices. For long gate length InP HEMTs, ΔV_T is negative and increasing in magnitude with decreasing L_g. At a certain L_g, however, there is a sign reversal and H-induced ΔV_T becomes positive.

In this work, we present a model for H-induced piezoelectric effect in InP HEMTs and GaAs PHEMTs that explains the peculiar behavior of ΔV_T shown in Fig. 1. Our model sheds light on the key parameters of the problem and provides design guidelines for minimizing H sensitivity of these devices.

II. Model

Our modeling approach involves: i) performing two-dimensional mechanical stress simulations, ii) computing the resulting piezoelectric charge in the semiconductor heterostructure, and iii) estimating its effect on V_T.

First, a 2D finite-element simulation tool, ABAQUS, was used to calculate the mechanical stress in the device layer structure introduced by an expanding gate. We modeled the expansion of the gate caused by the formation of TiH_x platelets as a thermal expansion of one of the layers of the multi-layer gate structure. We used a finer mesh near the surface and under the gate to provide a detailed picture of the mechanical stress where it has the biggest impact on V_T. We have exploited the symmetry of the structure and we only simulated half of it.

0-7803-6700-6/01/$10.00 ©2001 IEEE

Second, we use the atomic displacements u_x and u_z perpendicular and parallel to the gate, respectively, provided by ABAQUS to compute the polarization vector field and the polarization charge distribution throughout the device [6]. The x and z components of the polarization vector for a device on a [011] surface are respectively given by:

$$P_x = -\mu\, d_{14}\left(\frac{du_x}{dz} - \frac{du_z}{dx}\right)$$

$$P_z = -\mu\, d_{14}\frac{du_x}{dx}$$

In these equations μ is the Voight average shear modulus and d_{14} the piezo-electric constant of the material [7-10]. The values of these constants for the ternary compounds were obtained by interpolation. The piezo-electric charge can be calculated using:

$$\rho_{pol} = -\nabla \cdot P$$

The final step is to compute the effect of the polarization charge on V_T. For simplicity, we assume a 1D model in which ΔV_T is calculated at the center of the gate. This is a fair assumption particularly if V_T is experimentally extracted in the linear regime. In our V_T model, we assume that the Fermi level is pinned at the bottom of the buffer layer.

Applying electrostatics we find that:

$$\Delta V_T = -\int_{\substack{insulator\\channel}} \frac{1}{\varepsilon} P_z dz + \frac{1}{z_b}\left(\frac{z_i}{\varepsilon_i} + \frac{z_c}{\varepsilon_c}\right)\int_{buffer} P_z dz$$

In this equation, z_i and z_c are the thicknesses of the insulator and the channel layer, respectively, and z_b is the thickness of the buffer layer. We assume Fermi level pinning at the buffer/substrate interface. ε_i and ε_c are the permittivities of the insulator and the channel, respectively.

Our model suggests that ΔV_T is roughly proportional to the *difference* between the average of P_z above the channel and in the buffer layer. Because of this, all aspects of the heterostructure design are important, including the thickness of the buffer layer.

III. Results

As a model device (Fig. 2), we have selected a double-heterostructure transistor with a 300Å insulator layer and a 200Å channel. The gate is a 250Å Ti/ 250Å Pt/3000Å Au stack, surrounded by 600Å of Si_3N_4. Table 1 shows the different material constants that were used in this study. The mesh extends by 20 μm in the vertical direction and 50 μm in the horizontal direction from the center of the gate.

First, the 2D finite-element simulation tool yields atomic displacements everywhere in the heterostructure (Fig. 3). This information is used to calculate the corresponding piezo-electric charge distribution in the device (Fig. 4).

Our model for ΔV_T requires P_z at the center of the gate. This is shown in Fig. 5 for a 1 μm InP HEMT and GaAs PHEMT. The large change of P_z in the channel occurs because of the change in the material constants between channel and insulator.

Fig. 6 shows calculations of ΔV_T for both InP HEMTs and GaAs PHEMTs of different L_g and buffer thickness. These calculated values show a similar dependence on the gate length as the experimental observations in Fig. 1. For identical conditions, GaAs PHEMTs show a larger ΔV_T than InP HEMTs, as the piezo-electric constants are larger. Both types of HEMTs exhibit a similar change of ΔV_T as a function of the gate length. Long devices exhibit a negative V_T shift, while submicron devices show a positive V_T shift. This stems from the relative polarization constants of the insulator and channel that for the same stress yield a polarization in the channel that is much smaller than that in the buffer and insulator. As a result, for medium and long gate lengths, when the stress in the vertical direction of the structure exhibits a fairly soft distribution in depth, the average polarization in the buffer layer is higher than that in the insulator/channel layer structure. In consequence, ΔV_T is negative. For short channel devices, the stress sharply peaks directly underneath the gate, and the polarization in the buffer becomes relatively less relevant. In consequence, ΔV_T becomes positive.

Fig. 6 also shows that the buffer thickness, or the point where the Fermi level is pinned, plays a critical role. When the pinning occurs closer to the channel, the gate length at which ΔV_T changes sign becomes shorter. For an unpinned back interface, the charges in the buffer are irrelevant and ΔV_T is positive for all L_g.

The point at which ΔV_T changes sign depends also on the details of the layer structure. If the insulator thickness decreases, the sign-change will occur for shorter devices (Fig. 7).

The design of the gate affects ΔV_T greatly. If the layers above the expanding Ti are more rigid, ΔV_T decreases and ΔV_T changes sign at shorter gate lengths. This is seen if the thickness of these layers increases or when a higher Young's modulus is set for these layers. Since the top of the gate is more rigid, it will absorb more of the stress caused by the expanding gate compared to the device layers underneath. This decrease of stress will result in a lower ΔV_T. We also found that thinning the Ti layer will decrease ΔV_T and make the gate length at which ΔV_T changes signs shorter. If we remove the nitride layer in our simulations, we find it lowers ΔV_T significantly at shorter gate lengths (Fig. 8). This makes sense since the nitride adds rigidity to the gate.

The results of our model hinge on the material constants that are used. Some of which are not well known. Nevertheless, this study is useful in that it reveals the key variables that impact hydrogen-induced ΔV_T in HEMTs.

IV. Conclusions

We have modeled the hydrogen-induced ΔV_T in InP HEMTs and GaAs PHEMTs using piezoelectric polarization charge theory. The modeling results are broadly consistent with experimental observations. The modeling study reveals that it is possible to mitigate this problem through careful design of semiconductor heterostructure and the gate structure. Our work suggests that it is possible to select a heterostructure design that is insensitive to hydrogen at a certain gate length.

Acknowledgements

The authors would like to acknowledge R. Blanchard for her help in building this model and S. Adachi for his help in finding the material constants of the different materials. This research was partially funded by NTT.

References

[1] J. A. del Alamo et al. TWHM 2000.
[2] R. Blanchard *et al.*, Electr. Dev. Lett. 20, 8 (1999).
[3] P. Chao et al., IEEE Electr. Dev. Lett. 15, 5 (1994)
[4] R. Blanchard et al., IPRM 2000.
[5] M. Chertouk et al., IEEE Electr. Dev. Lett., 21, 97 (2000).
[6] P. Asbeck et al., IEEE Trans. on Electron Dev. 31, 10 (1984).
[7] V. Chin, Solid-State Electron. 37, 1345 (1994).
[8] G. Arlt et al., Phys. Status Solidi 25, 323 (1968).
[9] K. Hubner, Phys. Status Solidi B 57, 627 (1973).
[10] K.-H. Hellwege et al., Landolt-Bornstein Numerical data and Functional Relationships: Elastic, Piezo-electric, Pyroelectric and Piezooptic Properties, Springer-Verlag, 1984.

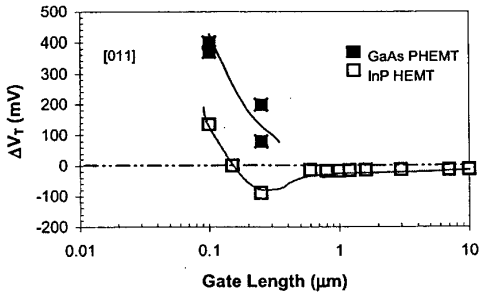

Fig. 1: Reported ΔV_T caused by hydrogen degradation as a function of gate length for InP HEMTs and GaAs PHEMTs with gates oriented along the [011] direction [2-5].

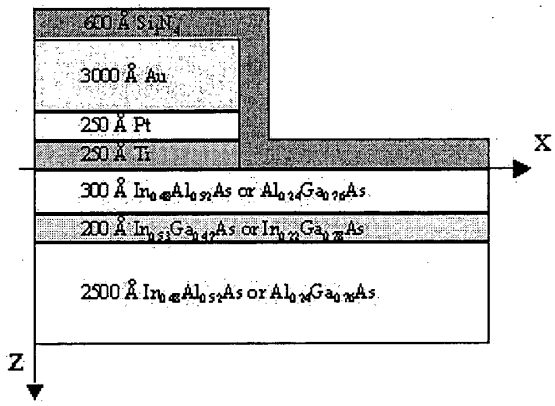

Fig. 2: Simulated device structures. Both the InP HEMT and GaAs PHEMT were simulated.

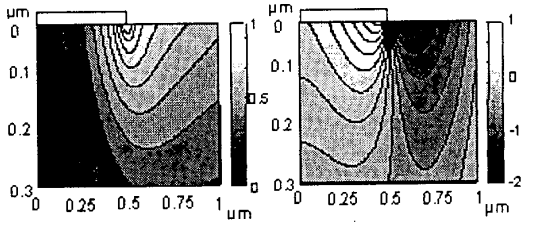

Fig. 3: Relative displacement parallel (left) and perpendicular (right) to the gate produced by an expanding gate in a 1 μm gate length HEMT. Calculations by ABAQUS. Only half of the structure is simulated.

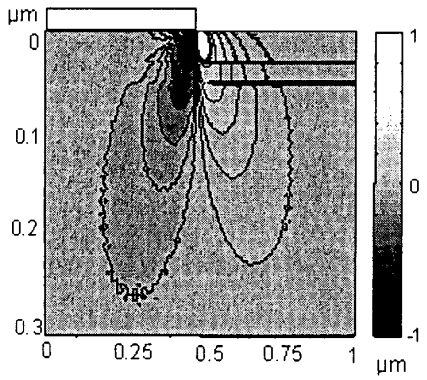

Fig. 4: Relative 2D piezoelectric charge distribution in a 1 µm HEMT stressed by an expanding gate.

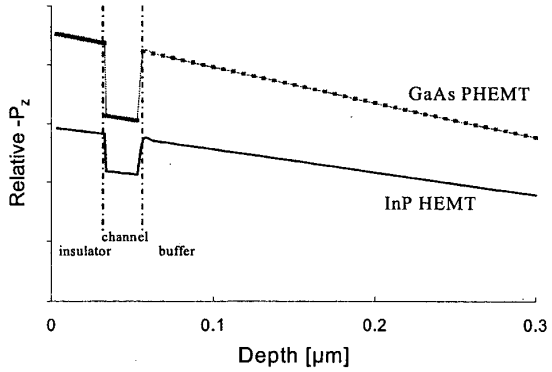

Fig. 5: Piezoelectric polarization vector in the direction perpendicular to the gate, P_z, for an InP HEMT and a GaAs PHEMT with 1 µm gate length.

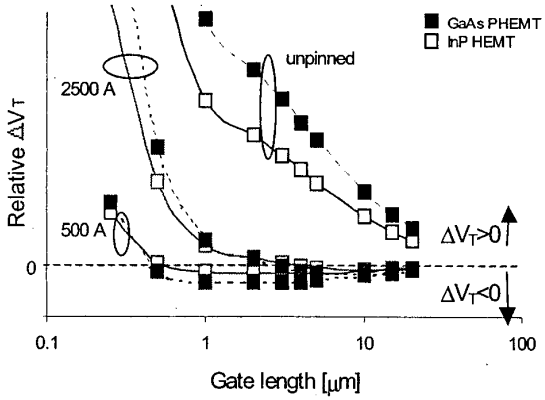

Fig. 6: Relative hydrogen-induced ΔV_T for InP HEMTs (solid lines) and GaAs PHEMTs (dashed lines) of different gate lengths. The different lines are calculations for different buffer layer thicknesses (with a pinned Fermi level at the buffer/substrate interface), as well as for an unpinned buffer/substrate interface.

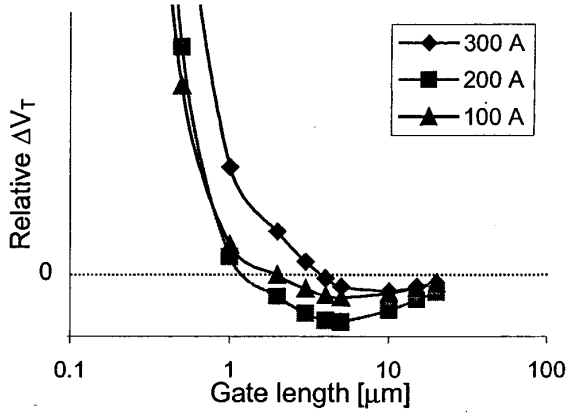

Fig. 7: Relative hydrogen-induced ΔV_T for InP HEMTs with insulator thicknesses of 100, 200 and 300 Å. The Fermi-level is pinned at the bottom of the buffer.

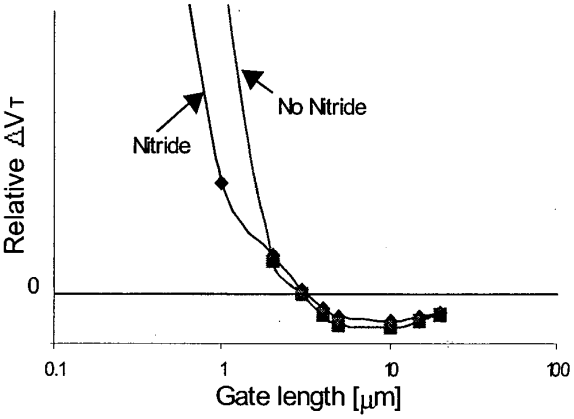

Fig. 8: Relative hydrogen-induced ΔV_T for InP HEMTs of different gate lengths. The Fermi-level is pinned at the bottom of the buffer.

Material	d_{14} [C/dyne]	µ [10^{10} dyne/cm^2]
GaAs	3.36 [7]	48.6 [10]
InAs	1.14 [8]	31.4 [10]
AlAs	5.00 [9]	44.2 [10]

Table 1: Material constants used in this study. The ternary compounds are linearly interpolated in between the binaries.