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A THEORETICAL ANALYSIS OF STRAIN IN GaN AND ITS EFFECTS ON CARRIER CONDUCTIVITY

Submitted to:

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December 1994

DEPARTMENT OF ELECTRICAL ENGINEERING

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UNIVERSITY OF VIRGINIA
School of Engineering and Applied Science

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13. ABSTRACT *(Maximum 200 words)*
We performed an ensemble Monte Carlo simulation of the electron transport in gallium nitride (GaN). Our calculation showed that intervalley electron transfer plays a dominant role in GaN in high electric fields leading to a strongly inverted electron distribution and to a large negative differential conductance. We found that, in a GaN-AlN-GaN SIS structure, the strain-induced electric fields can shift the flat band voltage and produce an accumulation region on one side and the depletion region on the other side of the AlN insulator. We used our theory, the current-voltage measurements and the capacitance-voltage measurements of the GaN-AlN-GaN SIS structures for quantitative characterization fo the degree of the AlN film relaxation depending on the film thickness. Our results show that the 30 Å AlN film is slightly relaxed, the 60 Å film data show well-developed relaxation process, and the 100 Å structure is almost fully relaxed. Out data indicate that the low bound of the conduction band offset for the AlN/GaN heterointerface is close to 1 eV.

14. SUBJECT TERMS
Gallium nitride, aluminum nitride, electron transport, semiconductor-insulator-semiconductor structures, elastic strain relaxation, piezoeffect, current-voltage characteristics.

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TABLE OF CONTENTS

I. The Electron Transport in GaN

We performed[1] an ensemble Monte Carlo simulation of the electron transport in gallium nitride (GaN). Our calculation showed that intervalley electron transfer plays a dominant role in GaN in high electric fields leading to a strongly inverted electron distribution and to a large negative differential conductance.

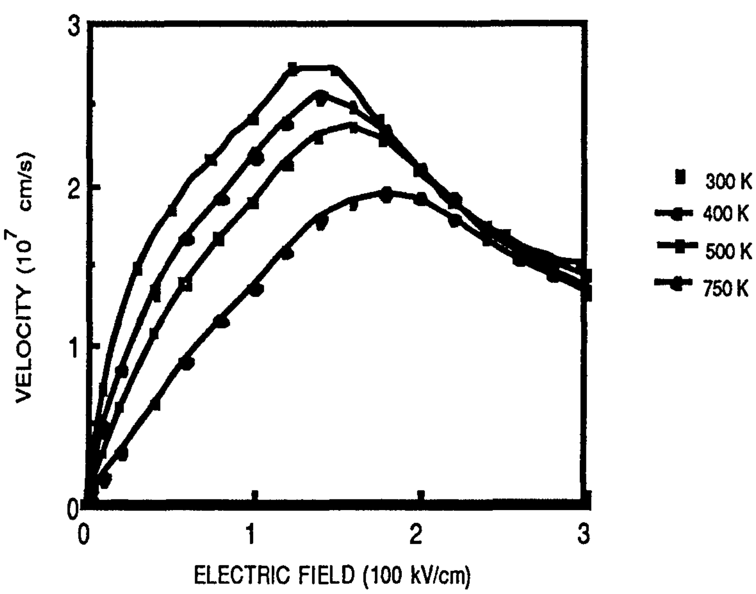

Figure 1. Electron Velocity in GaN as a Function of Electric Field for Different Temperatures.

We also derived an analytic expression for the polar optical momentum relaxation time for phonon energies larger than the thermal energy. This expression applies

[1]B. Gelmont, K. Kim, and M. Shur, J. Appl. Phys., 74, 1818 (1993)

to many wide-gap semiconductors, such as GaN and SiC, at room temperature since these semiconductors have large polar optical phonon energies (on the order of 100 meV). The calculated mobility agrees well with the results of the Monte Carlo calculation.

II. Charge Induced by Strain and C-V Characteristics in Wurtzite SIS Structures.

We calculated the strain-induced electric field and charge distribution in such structures[2,3]. We found that, in a SIS structure grown along a (0001) crystallographic direction, the strain-induced electric fields can shift the flat band voltage and produce an accumulation region on one side and the depletion region on the other side of the AlN insulator. The surface charge density caused by the piezoeffect is on the order of 10^{12} cm^{-2}. As a consequence of the asymmetry in the space charge distribution, the capacitance-voltage characteristics of the SIS structure become asymmetrical. The asymmetrical shift of the C-V characteristics with respect to the origin is on the order of 1.5 V for a 30 Å AlN film. This asymmetry should vanish in a relaxed film.

2 A. Bykhovski, B. Gelmont, and M. Shur , J. Appl. Phys., 74, 6734 (1993)
3 A. Bykhovski, B. Gelmont, and M. Shur , Appl. Phys. Letters, 63, 2243 (1993)

III. The Asymmetric C-V and the Elastic Strain Relaxation.

We used our theory and the capacitance-voltage measurements of the GaN-AlN-GaN SIS structures for quantitative characterization of the degree of the AlN film relaxation depending on the film thickness[4]. The starting point for the generation of misfit dislocation corresponds to $L \geq 30$ Å (see Fig. 2).

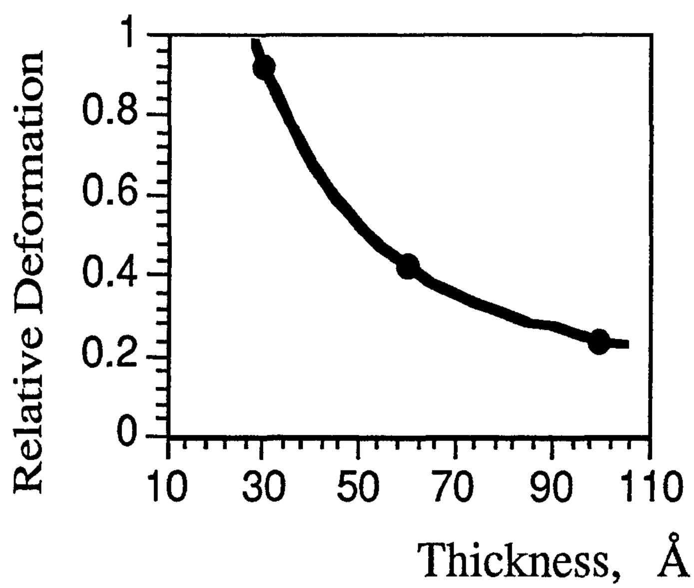

Figure 2. Relative Elastic Strain Tensor Component, $u_{xx}/u_{xx}(0)$, as a Function of AlN Thickness, L.
Here $u_{xx}(0)=(a_{GaN}-a_{AlN})/a_{AlN}$, a_i are lattice periods in the hexagonal plane. Circles are experimental data, solid line is interpolation. $N_d=2\cdot10^{17}$ cm^{-3}

This conclusion is in agreement with experimental studies of strained-layer GaN/AlN superlattices[5]. Our data show that the 75% elastic strain relaxation

[4] A. Bykhovski, B. Gelmont, M. Shur, and A. Khan, in: Proceedings of the International Conference on Silicon Carbide and Related Materials, Inst. of Phys. Conf. Ser. Number 137, Inst. of Physics Publishing, Bristol and Philadelphia, p 691 (1994).
[5] Sitar Z., Paisley M. J., Yan B., Ruan J., Choyke W. J., and Davis R. F., 1990, J. Vac. Sci. Technol., B 8, 316.

GaN/AlN superlattices[5]. Our data show that the 75% elastic strain relaxation takes place at L=100Å. The similar approach was applied to SiC/AlN/SiC SIS[6]. 2H(6H) SiC and wurtzite AlN were considered. We developed the characterization technique which can be used to determine the strains and (or) the doping concentrations from measured capacitance under zero bias.

[5]Sitar Z., Paisley M. J., Yan B., Ruan J., Choyke W. J., and Davis R. F., 1990, J. Vac. Sci. Technol., B 8, 316.

[6]A. Bykhovski, B. Gelmont, M. Shur, and M. Spencer, in: Proceedings of the International Semiconductor Device Research Symposium, Charlottesville, December 1-3, 1993, p. 581.

IV. GaN-AlN-GaN SIS: I-V Characteristics

We studied the elastic strain relaxation on the current-voltage (I-V) characteristics in SIS and estimated the AlN/GaN conduction band discontinuity from the measured I-V characteristics[7].

To calculate the current in forward direction, we assumed that electrons are first activated above the energy corresponding to the depletion layer barrier and then tunnel through the AlN layer. We obtained good agreement between the theory and the experiment for L = 100 Å assuming the uniform relaxation and found the low bound of AlN/GaN conduction band discontinuity at about 1 eV. We showed that the non uniformity of the film relaxation may have a dramatic effect on the current-voltage characteristics. We explained our experimental data for thinner AlN films in the frame of simple model which assumes just two regions with different degree of relaxation in order to account for the relaxational non uniformity across the device cross-section. The portion of the cross-section with a lower degree of relaxation determines the I-V characteristics at high bias and the portion of the cross-section with a higher degree of relaxation determines the I-V characteristics at low bias. Using our approach, we obtained satisfactory agreement with the experimental data (see Fig. 3).

Our results show that the 30 Å AlN film is slightly relaxed, the 60 Å film data show well-developed non-uniform relaxation process, and the 100 Å structure is almost fully and uniformly relaxed. In these films with L=30 Å - 100 Å the areas of weak and strong relaxation coexist. The upper limit for the elastic strain relaxation obtained using I-V is in a satisfactory agreement with the corresponding data obtained from the measured C-V of the same structures[4]. However, the I-V characteristics are more sensitive to the non-uniformity in the barrier energies than the C-V characteristics.

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[7] A. Bykhovski, B. Gelmont, M. Shur, and A. Khan, J. of Applied Physics., February (1995), to be published.

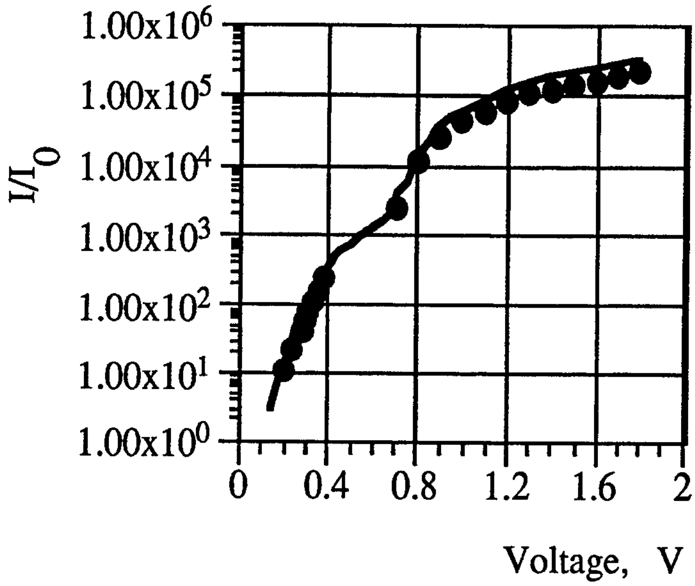

Figure 3. Forward Current in GaN-AlN-GaN SIS.
L= 30 Å.
Effective barrier is 0.9 eV; area is 31400 μm^2; series resistance is 10^5 Ω; donor concentration is $2x10^{17}$ cm^{-3} . I_0=0.034 nA, $j_0=I_0/S$= 1.08 mA/m^2. Solid line - calculations; points are experimental data.

V. Novel Pressure Sensor Based on GaN-AlN-GaN or SiC-AlN-SiC SIS

We proposed[8] a new sensor which is capable of operating at a very high temperature and has a large sensitivity. It can be fabricated using SiC-AlN-SiC or GaN-AlN-GaN Semiconductor-Insulator-Semiconductor structures. The change in the applied pressure can result in decreasing (or increasing) the current through SIS structure due to piezoeffect (see Fig. 4).

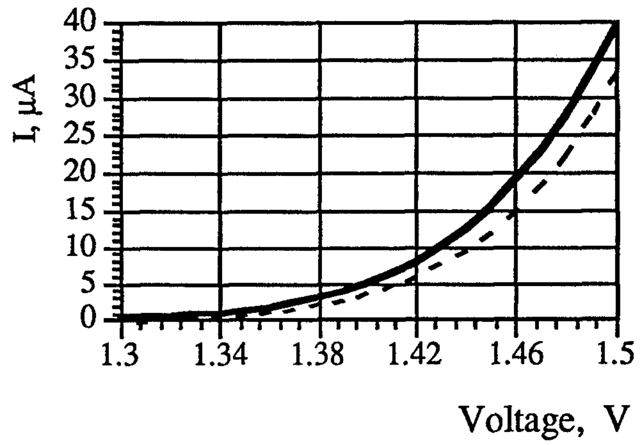

Figure 4. Forward Current Through the SIS Structure as a Function of Voltage.
Solid line: I-V without external pressure;
Dashed line: force 0.01 N applied to the surface of SIS.
Doping level is 2×10^{17} cm^{-3} . Area is 100 μm^2, series resistance is 10^3 Ω.

Applied pressure creates elastic strain in the barrier layer, which, in turn, changes the strain-induced electric field and, therefore, the shape of the barrier. The sensitivity of the device can be optimized by changing doping levels, a series resistance, temperature, the thickness of the barrier layer and the composition.

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[8] A. Bykhovski, M. Shur, and M. Spencer, Jan. 1994.

ABSTRACT:

"MONTE CARLO SIMULATION OF ELECTRON TRANSPORT IN GALLIUM NITRIDE" by B. Gelmont, K. Kim, and M. Shur.

The results of an ensemble Monte Carlo simulation of the electron transport in gallium nitride (GaN) are presented. The calculation shows that intervalley electron plays a dominant role in GaN in high electric fields leading to a strongly inverted electron distribution and to a large negative differential conductance. An analytic expression for the polar optical momentum relaxation time for phonon energies larger than the thermal energy is also derived. This expression applies to many wide-gap semiconductors, such as GaN and SiC, at room temperature since these semiconductors have large polar optical phonon energies (on the order of 100 meV). The calculated mobility agrees well with the results of the Monte Carlo calculation.

ABSTRACT:

"CURRENT-VOLTAGE CHARACTERISTICS OF STRAINED PIEZOELECTRIC STRUCTURES" by A. Bykhovski, B. Gelmont, M. Shur, and A. Khan, Journal of Applied Physics, to be published.

We present experimental and theoretical studies of the current-voltage characteristics of symmetrically doped n-type GaN-AlN-GaN Semiconductor-insulator-semiconductor (SIS) structures. The asymmetry caused by the strain-induced electric field leads to the depletion layer barrier in addition to the barrier presented by a thin insulating layer of AlN. We show that the tunnel current depends on the degree of the elastic strain relaxation which, in turn, is related to

the AlN film thickness, and that this dependence provides quantitative information about the film relaxation. This characterization technique is compared with the capacitance-voltage characterization of the SIS structures. Our data indicate the low bound of conduction band discontinuity of about 1 eV at AlN/GaN heterointerface.

ABSTRACT:

"THE INFLUENCE OF THE STRAIN-INDUCED ELECTRIC FIELD ON THE CHARGE DISTRIBUTION IN GaN-AlN-GaN STRUCTURE" by A. Bykhovski, B. Gelmont , and M. Shur published in Journal of Applied Physics,.74, 6734 (1993).

We show that strongly pronounced piezoelectric properties play a key role in GaN-AlN-GaN Semiconductor-Insulator-Semiconductor (SIS) and related structures. In sufficiently thin AlN layers, the lattice constant mismatch is accommodated by internal strains rather then by the formation of misfit dislocations. These lattice-mismatch-induced strains generate polarization fields. We demonstrate that, in a GaN-AlN-GaN SIS structure with the growth axis along a (0001) crystallographic direction, the strain-induced electric fields can shift the flat band voltage and produce an accumulation region on one side and the depletion region on the other side of the AlN insulator. Which side of the insulator the accumulation region is produced at, depends on the type of the atomic plane at the heterointerface (Ga or N). The surface charge density caused by the piezoeffect is on the order of 10^{12} cm^{-2}. As a consequence of the asymmetry in the space charge distribution, the capacitance-voltage characteristics of the SIS structure become asymmetrical. The asymmetrical shift of the C-V characteristics

with respect to the origin is on the order of 1.5 V for a 30 Å AlN film. This asymmetry should vanish in a relaxed film. Hence, the capacitance-voltage measurements of the GaN-AlN-GaN SIS structures can be used for quantitative characterization of the degree of the AlN film relaxation depending on the film thickness. This and related techniques should become an important tool for the characterization of piezoelectric layered semiconductor films.

ABSTRACT:

"STRAIN AND CHARGE DISTRIBUTION IN GaN-AlN-GaN SEMICONDUCTOR-INSULATOR-SEMICONDUCTOR STRUCTURE FOR ARBITRARY GROWTH ORIENTATION" by A. Bykhovski, B. Gelmont, and M. Shur , Appl. Phys. Letters, 63, 2243 (1993).

We demonstrate that, in a GaN-AlN-GaN Semiconductor-Insulator-Semiconductor (SIS) structure, the strain-induced electric fields across the interface depend on the angle, θ, between the c-axis and the growth direction. The magnitude of the strain induced polarization has a maximum in (0001) crystallographic direction ($\theta=0^{o}$) and a subsidiary maximum near $\theta=70^{o}$. This angular dependence is a unique feature of wurtzite-type structures. Considering θ as an independent parameter for device design, one can obtain structures with flat band voltage shift from 0 to 1.5V for 30Å AlN film, with different positions of accumulation-depletion regions, and with electron (hole) charge varying from 0 to more then 10^{12} cm^{-2}.

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