OFFICE OF NAVAL RESEARCH
PUBLICATION/PATENTS/PRESENTATIONS/HONORS REPORT
1 Oct 93 through Sep. 30 1994

R&T Number: 414s014---02
Contract/Grant Number: N00014-92-J-1580/P00001
Contract/Grant Title: Comparative Study of GaN and SiC
Principal Investigator: Michael Shur
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Papers Submitted to Referred Journals:


Papers Published in Referred Journals:


Books and Chapters:

None.

Printed Tech. Reports & Non-Referred Papers:


Invited Presentations:


Presentations:


Honors and Awards:

Graduate Students and Post-Docs Supported:

1 Senior scientist, and two post-docs (Two white males and one Asian male)
I. The Electron Transport in GaN

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

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. 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

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piezoeffect is on the order of $10^{12} \text{ cm}^{-2}$. 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.

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). This conclusion is in agreement with experimental studies of strained-layer GaN/AlN superlattices$^5$. Our data show that the 75% elastic strain relaxation takes place at $L=100$ Å. 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.

IV. GaN-AlN-GaN SIS: I-V Characteristics
We studied the elastic strain relaxation on the current-voltage (I-V) characteristics in SIS and determined 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
estimated the 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. However, the I-V characteristics are more sensitive to the
non-uniformity in the barrier energies than the C-V characteristics.

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

\[8\text{A. Bykhovski, M. Shur, and M. Spencer, Jan. 1994.}\]
The change in the applied pressure can result in decreasing (or increasing) the current through SIS structure due to piezoeffect (see Fig. 4). 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.
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:

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 conduction band discontinuity of about 1 eV at AlN/GaN heterointerface.

ABSTRACT:
"THE INFLUENCE OF THE STRAIN-INDUCED ELECTRIC FIELD ON
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 than 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:

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, $\theta$, between the c-axis and the growth direction. The magnitude of the strain induced polarization has a maximum in (0001)
crystallographic direction (θ=0°) and a subsidiary maximum near θ=70°. 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 than 10^{12} cm^{-2}. 