

Theoretical study of pH response of electrolyte AlGaN/GaN ion sensors

Michael Bayer, Christian Uhl, Stefan Birner¹ and Peter Vogl

The concept of detecting salt concentrations and charged bio-molecules by semiconductor devices has stimulated a rapidly growing field of semiconductor based ion sensors. Requirements for physiological applications of such devices are chemically inert oxide surfaces and non-toxic materials. Thus a highly promising material system is $\text{Al}_x\text{Ga}_{1-x}\text{N}$ that additionally is extremely sensitive to changes of the surface charge or surface potential due to its high piezo and pyroelectric fields. We developed a model to explain and predict the sensitivity of solution gate AlGaN/GaN field effect transistors (FET) to charged adsorbates at the semiconductor/electrolyte interface that are controlled by the pH value of the electrolyte. Invoking the site-binding model for the chemical reactions at the oxidic semiconductor-electrolyte interface and taking into account strain, deformation potentials and the piezo and pyroelectric polarizations that result in interfacial sheet charge densities within the nitride heterostructure (Fig. 1), the spatial charge and potential distribution have been calculated self-consistently both in the semiconductor and the electrolyte. In addition, we calculated the source-drain current and its sensitivity to the electrolyte's pH value.

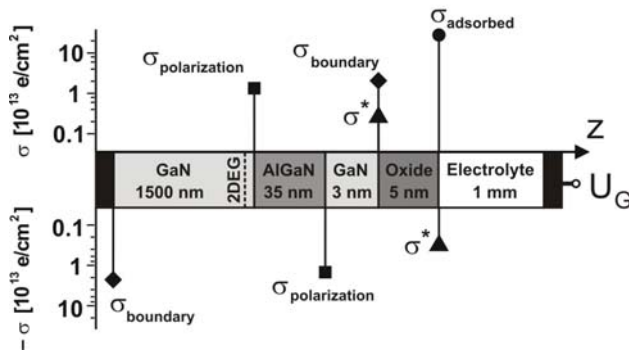


Fig. 1:

Schematic layout of the calculated heterostructure (Ga-face polarity) where the electrolyte is placed on top of a Ga oxide. The interface charge densities and their magnitudes in units of 10^{13} e/cm^2 are indicated by closed symbols and the axis to the left. A gate voltage U_G can be applied to the electrolyte. The position of the 2DEG is indicated.

The charge distribution at any point within the electrolyte solution that may contain several different types of ions is governed by the potential (Fig. 2) that is determined by the Poisson-Boltzmann equation, involving the valency and concentration of each ion species. Because of adsorption or desorption of hydrogen ions at oxide surface sites, the oxide/electrolyte interface gets either positively or negatively charged. To calculate this charge, the site-binding model for amphoteric surfaces was employed. Here, hydroxyl groups at the surface sites get either protonized or deprotonized. The adsorbed oxide/electrolyte interface charge σ_{adsorbed} depends on two dissociation constants for describing the surface reactions, the pH value of the electrolyte and the potential at the oxide/electrolyte interface. Experimental results were used to determine the values of the relevant dissociation constants and the concentration of the sites on the oxide. We varied the pH value of the electrolyte solution and calculated the adsorbed surface charges (Fig. 3a) which influence the electrostatic potential and thus the spatial variation of the conduction band edge. The huge piezo and pyroelectric polarization fields lead to the formation of a two-dimensional electron gas (2DEG) as indicated in Fig. 1 with an integrated sheet density of the order of 10^{13} cm^{-2} . The relevant part in the semiconductor is the density of the 2DEG that responds sensitively to changes in the electrolyte, i.e. changes in the pH value.

¹phone:+49-89-289-12752, fax:+49-89-12737, email: stefan.birner@nextnano.de

We calculated the 2DEG density (Fig. 3b) and the source-drain current of this AlGaIn/GaN FET parallel to the interface as a function of the surface charge density that arises from chemical reactions at the Ga oxide layer that is exposed to the electrolyte.

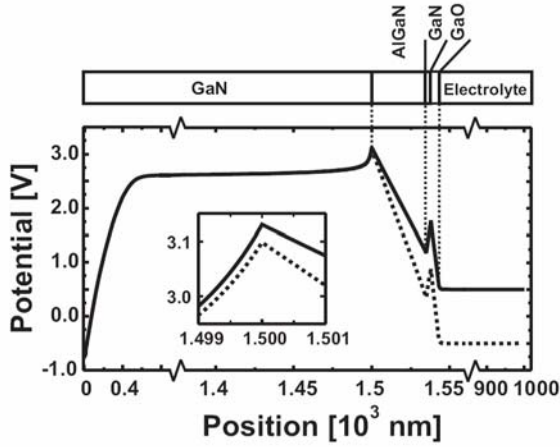


Fig. 2:

Spatial potential distribution for the entire structure with an electrolyte of pH=5.3 as calculated by the Poisson-Boltzmann equation. Depicted are the cases for an electrolyte gate voltage of $U_G=0.5$ V (solid line) and $U_G=-0.5$ V (dotted line), respectively. The inset shows a blow-up of the potential near the position of the 2DEG and illustrates the effect of an externally applied bias.

In order to reproduce recent experimental results we had to take into account an additional charge σ^* (Fig. 1) at the inner oxide surface that is essential for the sensitivity of the device because it effects the 2DEG density. Since experiments on the oxide growth on GaN have indicated voids in the oxide surface, some of the adsorbed ions can reach the inner oxide surface. The best agreement with the experimentally obtained I-V curve was obtained by assuming this charge to be 2% of the actual oxide/electrolyte interface charge. Our model can be used to enhance the efficiency of the sensor systematically by increasing the oxide thickness or by decreasing the Al mole fraction in the AlGaIn layer. For a structure of N-face polarity, we found that the response of the 2DEG density to changes in the pH value as well as the applied voltage is larger and provides a more efficient control of the device. Our calculations show a significant enhancement in the variation of the 2DEG density as a function of the pH value as compared to the Ga-face structure. All computations have been carried out using the nano device simulation tool **nextnano³** [1].

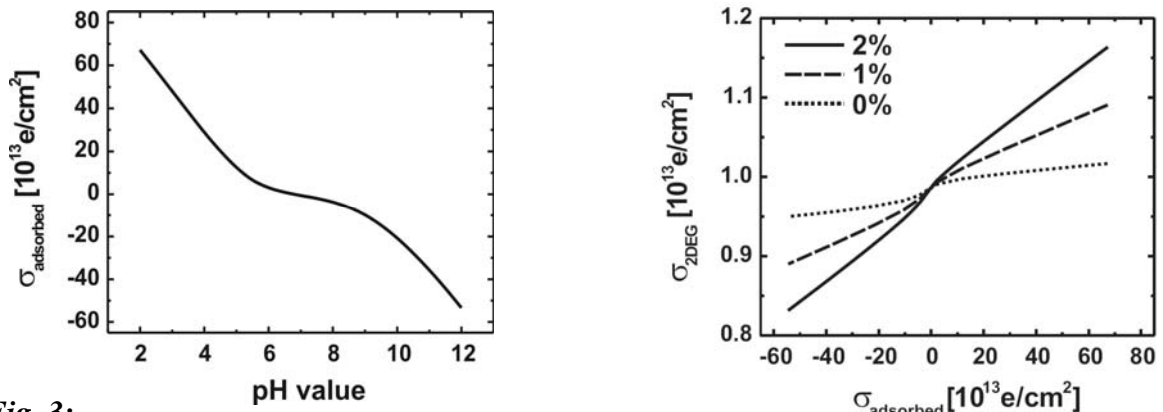


Fig. 3:

a) Calculated variation of the oxide/electrolyte interface charge density σ_{adsorbed} of the amphoteric surface with the pH value. As one can see, there is a range of pH values where the net surface charge is close to zero. Nevertheless, within this range the 2DEG density still varies as it also depends on the surface potential.

b) The 2DEG density as a function of the interface charge σ_{adsorbed} for different values of σ^ .*

[1] The **nextnano³** software package can be downloaded from www.wsi.tum.de/nextnano3. Support is available through www.nextnano.de.