

Simulation Standard

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Simulating the Source of Polarization Charge in AlGaIn/GaN HFETs

Polarization-induced charges at the AlGaIn/GaN interface of heterojunction field-effect transistors (HFETs) create a high density, two-dimensional electron gas (2DEG) in the channel. One approach to simulating the 2DEG is to place a fixed positive charge at the AlGaIn/GaN interface, thus attracting a fixed quantity of electrons to the channel. Silvaco's *ATLAS* software can do this with either an INTERFACE statement or automatically with the use of the POLARIZATION parameter on the REGION statement. This is fine, as far as it goes, but this simple approach glosses over some nuances having to do with the source of carriers in the channel. A paper by Ibbetson, *et al.*, [1] explored this question theoretically and experimentally. Based on an analysis of the electrostatics of the structure, they determined that surface states at the top of the AlGaIn barrier are the most likely source of the electrons attracted to the channel. This article demonstrates the simulation of this effect.

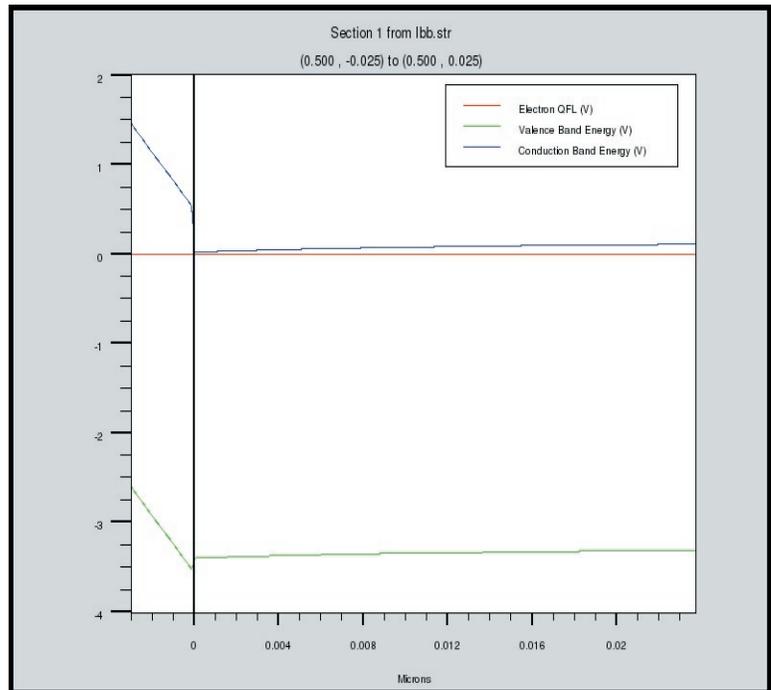


Figure 1. Band diagram of 30 Å of AlGaIn on GaN.

Ibbetson gave two possible explanations of the mechanism by which charge is transferred from the surface donor states to the 2DEG. Our simulations support his second explanation, that of surface pinning of the Fermi level. In wurtzite materials, the polarization has a spontaneous and a piezoelectric component. It is assumed that the relatively thick GaN buffer layer is unstrained, so it has only the spontaneous component. So fixed charges for GaN, $2.122 \times 10^{13} \text{ cm}^{-2}$, are placed at the top ($-2.122 \times 10^{13} \text{ cm}^{-2}$) and bottom ($+2.122 \times 10^{13} \text{ cm}^{-2}$) of the buffer layer. The thin AlGaIn layer is assumed to experience a uniform strain from its composition-dependent lattice mismatch with the GaN substrate. For the 34% AlN composition of AlGaIn used in Ibbetson's experiments, the nominal value of the total polarization charge is $4.005 \times 10^{13} \text{ cm}^{-2}$, so $-4.005 \times 10^{13} \text{ cm}^{-2}$ is placed at the top surface of the AlGaIn and $+4.005 \times 10^{13} \text{ cm}^{-2}$

cm^{-2} is placed at the bottom, at the interface with GaN. Therefore, the total polarization charge placed at the interface is $+1.883 \times 10^{13} \text{ cm}^{-2}$, which would attract that density of electrons to the 2DEG in the channel. That is not

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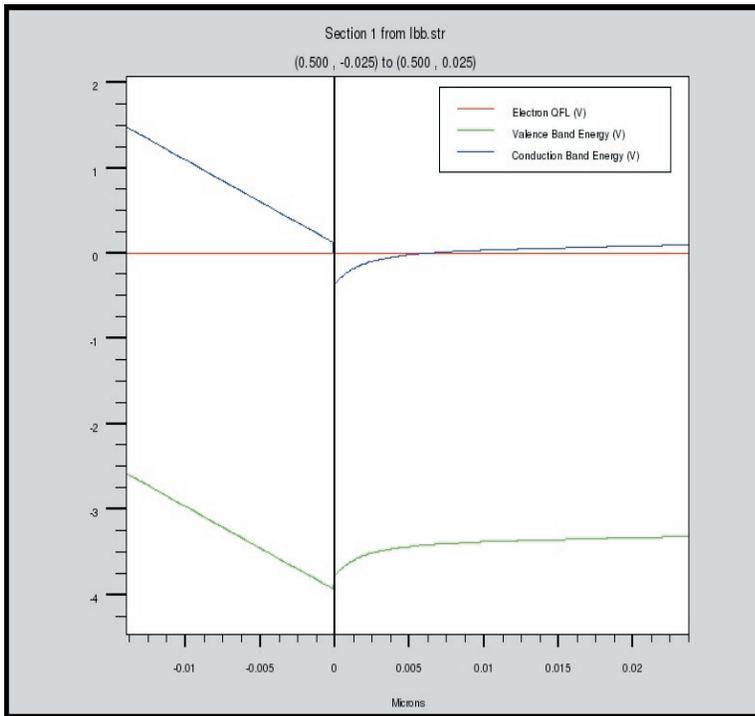


Figure 2. Band diagram of 140 Å of AlGaIn on GaN.

exactly the density value actually found for the 2DEG. The density of the 2DEG varies with the thickness of the AlGaIn layer.

Figures 1 and 2 show that the Fermi level at the AlGaIn surface is pinned at 2.6 volts above the valence band by the presence of the donor traps and the polarization charge. In Figure 1, the thickness of the AlGaIn is 30 Å. In this case, the Fermi level is below the GaN conduction band, so no accumulation of charges occurs in the channel.

In Figure 2, the thickness of the AlGaIn layer is 140 Å, and the Fermi level is above the GaN conduction band at the interface, creating a depletion region in which electrons may accumulate to form the 2DEG.

In order to match Ibbetson's measured results, we adjusted three variables: the ionization energy of the donor surface traps, the magnitude of the AlGaIn polarization charge, and the density of the surface traps. The surface trap density had to exceed that of the surface polarization charge. This was done in *ATLAS* with the help of the *DeckBuild* design of experiments tool, Batch DOE. Figure 3 overlays our simulated (red) and the measured (green) results.

Conclusion

In conclusion, understanding and controlling the source of the electrons in the 2DEG in AlGaIn/GaN HFETs is important for the optimization of their performance. The Silvaco toolset has shown itself to be useful in this regard.

References:

- [1] Ibbetson, J.P., *et al*, "Polarization Effects Surface States, and the Source of Electrons in AlGaIn/GaN Hetrostructure Field Effect Transistors", *Appl. Phys. Lett.*, V.77, N.2, 10 July 2000, pp. 250-252.

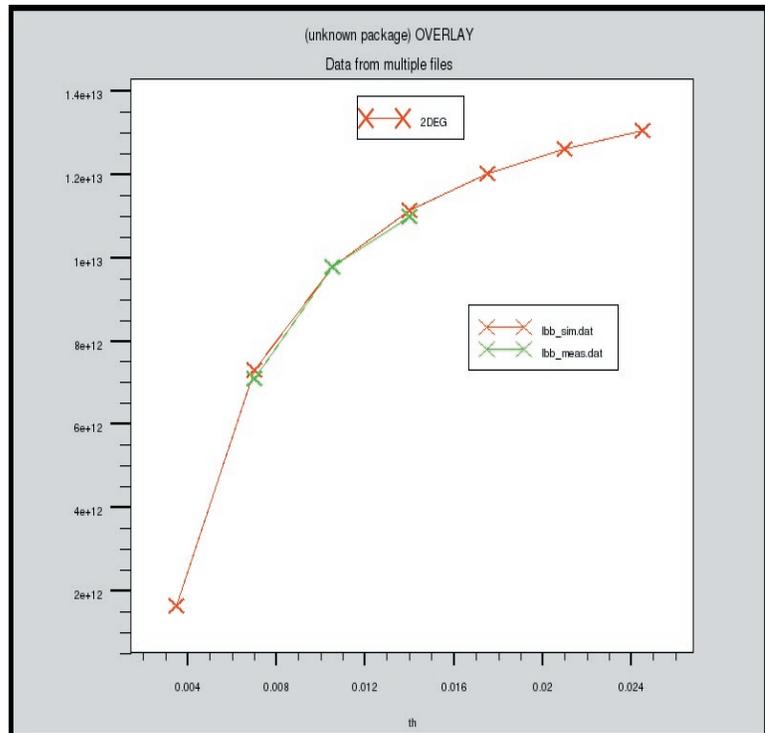


Figure 3. 2DEG density versus AlGaIn barrier thickness.