Correct Treatment of Spontaneous Polarization at Polar Wurtzite Interfaces

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Herbert Kroemer's famous statement, "the interface is the device," also applies to polar interfaces in nitride-based devices; but in wurtzite-structure materials we additionally have to reckon with polarization fields. Sometimes these fields are a nuisance, suppressing efficiency of light emitters, sometimes they provide functional enhancement, by increasing the density of two-dimensional carrier gases in transistors. Accurate knowledge of polarization constants is critical for analysis of experiments and for device design. Some time ago we identified deficiencies in the calculation of polarization fields in simulation tools, related to the choice of the zinc-blende phase as a reference for the spontaneous polarization of wurtzite [1]. However, since the current implementations contain *two* errors that to some extent cancel, most modeling has continued to use the zinc-blende-referenced approach. This has, unfortunately, led to major confusion in the analysis of polarization in AlScN alloys. Correct referencing of spontaneous polarization (relative to a layered-hexagonal phase) is essential for consistent interpretation of ferroelectricity [2,3].

Correct referencing of polarization also allows for an intuitive visualization of the origins of polarization, in which the electron cloud within the unit cell is shifted relative to the positive ionic cores. Different shifts in GaN and (strained) AlN then produce the polarization discontinuity at the interface, and lead to the insight that the electrons in the two-dimensional electron gas (2DEG) at a GaN/AlN [0001] heterojunction are *intrinsic* to the interface; i.e., they do not need to be provided by doping or surface states [4]. The surface actually acts as a *sink* for electrons; proper surface engineering should prevent interfacial carriers from leaking away to the surface. The majority of the compensation charge on the surface is provided by fixed charge [5]. This is consistent with the observation that the density of surface states (containing mobile charge) is much lower than the 2DEG density [6]. All these considerations also apply, *mutatis mutandis*, to hole gases at GaN/AlN [000-1] junctions.

Work performed in collaboration with Cyrus Dreyer, Haochen Wang, Sai Mu, Nicholas Adamski, Suhyun Yoo, Darshana Wickramaratne, Mira Todorova, Jörg Neugebauer, and Simon Fichtner, and supported by DOE, SRC, and ARO.

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