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Polarization Effects in III-N Semiconductor Devices

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1. Introduction

The correct microscopic foundations of dielectric polarization theory have only been established in the present decade. Remarkably, insights from that theory have recently come to bear quite heavily on the very practical field of endeavour of optoelectronic and electrical devices based on III-V nitrides, a class of semiconductors burgeoning in high-frequency and high-power applications.

III-V nitrides are a new frontier of semiconductor physics for several reasons. The one that concerns us here is polarization. It has recently been realized that the bulk macroscopic polarization properties of wurtzite III-V nitrides are largely unprecedented among semiconductors of applicative importance; indeed, unlike zincblende compounds such as GaAs, they exhibit a large *spontaneous* polarization (a token of their low-symmetry crystal structure) as well as larger-than-usual piezoelectric coupling constants. Large polarizations can thus exist in both unstrained and strained nitride layers. As expected from electrostatics, polarization changes at nitride heterointerfaces result in (localized, fixed, and invariable) interface charges with typical densities way above 10^{13} cm^{-2}: as a consequence, huge built-in electrostatic fields are generally present in the active regions of nitride quantum-confinement devices and heterostructures. It is therefore obvious that polarization affects dramatically the optical and electrical properties of multilayered nanostructures, and thus optoelectronic as well as electrical devices.

The main observable effects reported so far include "built-in" quantum-confined Stark effects, i.e. red shifts of transition energy and concurrent suppression of oscillator strenghts in MQWs for increasing well thickness; "piezodoping", i.e. the generation of high-density 2DEG at heterointerfaces due to polarization fields (indeed, this is not at all a purely piezoelectric effect); unusual excitonic effects due to the coupled fields in superlattice barriers and wells; blue shifts of the transition energies and attendant recovery of oscillator strength in MQW's under intense photoexcitation or injection; in connection to the latter, unusually high lasing thresholds.

2. Consequences of polarization

We cannot address all these issues here (see however the reference list), so we will only briefly discuss a few key points on the polarization-related properties of nitride systems.

Field patterns in heterostructures

A point which has generated confusion lately is the field pattern (i.e. values, signs, etc.) in the various layers of multi-interface stuctures (superlattices, HEMTS, MQWs, ...). Whatever the origin of the polarization fields (see below), key point n.1 is that only polarization *differences* between layers matter (i.e. produce electric fields), not absolute values in one or the other layer. Key point n.2 is that geometric parameters, such as layer thicknesses, also concur to determine the field pattern when the barrier and well thicknesses are both finite. Hence the field pattern is determined by all the layers and interfaces present in the whole structure. It is then vital to keep in mind that the indirect determination of fields (by PL, CV profiling, etc.), hence the assessment of their origin, should rely on simulations of the whole structure, and not, say, of the single active QW or heterointerface. [For example, a single QW between "infinite" barriers has approximately twice the internal field as the same QW embedded in a superlattice with equal-thickness barriers and wells. Of course, intermediate situations must be sorted out case by case.]

Spontaneous vs. piezoelectric polarization

So far, the existence of spontaneous (or intrinsic) polarization (SP) has not been widely accepted in this field. Indeed, however, SP does exist, and it makes a large difference in the field values expected in devices. That is because SP has a *fixed* direction and depends on composition, but *not* on strain; piezoelectricity, by contrast, depends on both composition and strain, and can point in any direction.

A couple of trivial consequences: AlGaN/GaN based systems are dominated by SP fields due to the large SP difference with GaN, while InGaN/GaN systems are dominated by piezoelectricity, as SP is almost the same in InN and GaN; Fully relaxed layers, whereby piezoelectricity is absent, are nevertheless polarized because of SP; The neglect of SP often yields incorrect signs of the fields, messing up the picture when analyzing e.g. the formation of 2DEGs in heterostructure HEMTs (e.g. "piezodoping"), or band offsets between polarized overlayers. [Interpretations only accounting for piezoelectricity typically contain combinations of errors in the patterns of polarization and electrostatic fields in the structures, and of uncertainties in polarity, piezoconstants, and strain relaxation. Things are clearing up more and more as these latter issues are addressed.]

A highly non-trivial consequence is that the existence of SP allows to remove polarization altogether, combining it appropriately with piezoelectricity by proper design and judicious choice of composition. This requires the use of either AlInN (of order 70 % Al) or AlGaInN (of order 10 % Al and 4 % In) alloys.

Screening: polarization vs excitation and doping

Real devices contain intrinsic, extrinsic, photoexcited, or injected free carriers. Their interplay with polarization fields gives rise to remarkable effects. Except for thick wells, intrinsic carriers are irrelevant in MQWs [they are not, of course, in single heterostructures where they in fact pile up into a 2DEG at a preferred interface].

In optical experiments, or in electrically driven structures, extrinsic carriers become relevant at sufficient injection or excitation densities: indeed, (say) photogenerated holes and electrons are separated spatially by the field in the QW, and pile up near the interface walls, screening out (in part) the polarization charges on the respective sides. Two ingredients are essential here, *(a)* density and *(b)* localization length. *(a)* The density must be high enough to screen out the (fixed, and large) polarization charge; hence, only at very high excitation powers will screening be effective. This turns out to match quantitatively the unusually high lasing thresholds observed in real devices. *(b)* The localization length of the quantum confined states (≥ 20 Å) is normally much larger than that of the polarization charge (≤ 5 Å): since screening effectively occurs over the largest of these lengths, a region near the QW walls always remains subjected to field, and a spatial separation of electrons and holes survives even at high power. Therefore, the recombination probability never reaches that of a flat well, reducing quantum efficiency irredeemably. In a word, at high power the transitions are blue-shifted and the oscillator strength recovers, but not *quite* to the flat band values.

More issues in optical experiments: Excitonic effect are poorly understood so far, but qualitatively one expects field ionization at low power, and conversely exciton bleaching at high power, at least in single QWs, while MQWs and superlattices seem to exhibit coupled-well "oblique" excitons. Many body effects such as band-gap renormalization are non-negligible, but seem to have a relatively minor role.]

Extrinsic free carrier generation by photoexcitation (say) and the ensuing partial "rectification" of the well profiles is transient, while in a light-emitting device one would like to do it for good, and independently of injection. One way to do this is by remote doping, which provides the QW with extrinsinc charge to screen the polarization charge. The needed doping may range in the 10^{20} cm^{-3} for AlGaN/GaN, while about 10^{19} cm^{-3} is sufficient for typical InGaN/GaN systems.

Open issues

To avoid making this the longest section in this note, we restrict to a single task: The relative importance of spontaneous and piezoelectric polarization should be estimated quantitatively, and the two components measured. Among the many things that could be tried, we suggest
(a) optical experiments on carefuly designed *unstrained* AlGaInN MQWs to isolate SP;
(b) optical experiments on AlGaInN/GaN or AlInN/GaN MQWs designed so that SP and piezoelectricity cancel each other;
(c) electrical and CV measurements on HEMTs of known polarity and strain state, measuring 2DEG densities at interfaces.

To interpret experiments properly, simulations are typically needed, and it is essential that they use accurate ingredients. In particular, the polarity of the crystal should be known: this entails either ascertaining the role of mosaicity and polarization domains, or (preferrably) a direct polarity control, e.g. by polarity inversion by Mg treatment. Not least, piezoelectric constants should be measured accurately to check those available from theory, including their possible non-linearities.

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