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(Hopefully, this is a typo and should read Rome, Italy)

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Huge built-in electric fields have been predicted to exist in wurtzite III-V nitrides thin films and multilayers. Such fields originate from heterointerface discontinuities of the macroscopic bulk polarization of the nitrides. Here we discuss the background theory, the role of spontaneous polarization in this context, and the practical implications of built-in polarization fields in nitride nanostructures.

To support our arguments, we present detailed self-consistent tight-binding simulations of typical nitride QW structures in which polarization effects are dominant.

73.40.Kp, 77.22.Ej, 73.20.Dx

I. INTRODUCTION

Spontaneous polarization has long been known to take place in ferroelectrics. On the other hand, its existence in semiconductors with sufficiently low crystal symmetry (wurtzite, at the very least) has been generally regarded as of purely theoretical interest. Recently, a series of first principles calculations has reopened this issue for the technologically relevant III-V nitride semiconductors, whose natural crystal structure is, in fact, wurtzite. Firstly, it was shown that the nitrides have a very large spontaneous polarization, as well as large piezoelectric coupling constants. Secondly, it was directly demonstrated how polarization actually manifests itself as electrostatic fields in nitride multilayers, due to the polarization charges resulting from polarization discontinuities at heterointerfaces. This charge-polarization relation, counterchecked in actual ab initio calculations, has been exploited to calculate dielectric constants.

While piezoelectricity-related properties are largely standard, spontaneous polarization is to some extent new in semiconductor physics, to the point that, so far, the practical importance of spontaneous polarization in III-V nitrides nanostructures (multi quantum wells, or MQW’s, are the particular focus of this paper) has been largely overlooked. It is tantalizingly clear to us, however, that these concepts may lead to a direct and unambiguous measurement of the spontaneous polarization in semiconductors, to the recognition of its importance in nitride-based nanostructures, and, hopefully, to its exploitation in device applications. In the hope of accelerating these processes, in this paper we show how to account for the effects of spontaneous polarization in MQW’s, and discuss some prototypical cases and their possible experimental realization. To support our arguments, we present simulations of a typical AlGaN/GaN MQW where spontaneous and piezoelectric polarizations are about equal.

Among the consequences of macroscopic polarization which we will demonstrate in this paper let us mention the following: (a) the field caused by the fixed polarization charge, superimposed on the compositional confinement potential of the MQW, red-shifts dramatically the transition energies and strongly suppresses interband transitions as the well thickness increases; (b) the effects of thermal carrier screening are negligible in typical MQW’s, although not in massive samples; (c) a quasi-flat-band MQW profile can be approximately recovered (i.e. polarization fields can be screened) only in the presence of very high densities of free carriers, which are appreciably larger than those typical of semiconductor laser structures; (d) even in the latter case, transition probabilities remain considerably smaller than the ideal flat band value, and this reduces quantum efficiency; (e) once an appropriate screening density (i.e. the pumping power) has been chosen to ensure that the recombination rate is sufficient, a residual polarization fields is typically still present: this provides a means to intentionally red-shift transition energies by changing well thicknesses, without changing composition; (f) the very existence of distinct and separately controllable spontaneous and piezoelectric polarization components allows to choose a composition such that they cancel each other out, leading to very nearly ideal flat-band conditions. A fuller understanding of these points cannot be but helpful to the design of real nitride devices, and their operation, involving carrier generation by light, current injection, or doping.
II. PIEZOELECTRIC FIELDS

Piezoelectricity is a well known concept in semiconductor physics. Binary compounds of strategic technological importance like III-V arsenides and phosphides can be forced to exhibit piezoelectric polarization fields by imposing upon them a strain field.

Among others, applications of piezoelectric effects in semiconductor nanotechnology exist in the area of multi quantum wells (MQW) devices. A thin semiconductor layer (active layer) is embedded in a semiconductor matrix (cladding layers) having a different lattice constant. If pseudomorphic growth occurs, the active layer will be strained and therefore subjected to a piezoelectric polarization field, which can be computed as

\[ \text{D}^{(pz)} = \vec{\varepsilon} \cdot \vec{\varepsilon} \]  

(1)

if the strain field \( \varepsilon \) and the piezoelectric constants tensor \( \vec{\varepsilon} \) are known.

The existence of a polarization field in a finite system implies the presence of electric fields. For the piezoelectric case, the magnitude of the latter depends on strain, piezoelectric constants, and (crucially) on device geometry. The structure of a typical III-V nitride-based superlattice or MQW is \( \text{C} = \text{A} - \text{C} - \text{A} - \text{C} - \text{A} - \text{C} - \text{A} - \text{C} - \text{A} \) (A=active, C=cladding), where both the cladding layer and the active layer are in general strained to comply with the substrate in-plane lattice parameter. In such a structure, the electric fields in the A and C layers are

\[ \begin{align*}
E^{(pz)}_A &= 4\pi \ell_C (P^{(pz)}_C - P^{(pz)}_A) / (\ell_C \varepsilon_A + \ell_A \varepsilon_C) \\
E^{(pz)}_C &= 4\pi \ell_A (P^{(pz)}_A - P^{(pz)}_C) / (\ell_C \varepsilon_A + \ell_A \varepsilon_C)
\end{align*} \]  

(2)

where \( \varepsilon_{A,C} \) are the dielectric constants and \( \ell_{A,C} \) the thicknesses of layers A and C. Thus, in general, an electric field will be present whenever \( P_A \neq P_C \). The above expressions are easily obtained by the conditions that the electric displacement be conserved along the growth axis, and by the boundary conditions that the potential energy on the far right and left of the MQW structure are the same.

There are essentially three special cases of MQW structures worth a mention:

i) active (cladding) layer lattice matched to the substrate: \( P_A = 0 \) (\( P_C = 0 \));

ii) \( \ell_A = \ell_C \), whence \( E_A = -E_C \);

iii) \( \ell_A \ll \ell_C \), implying \( E_C \simeq 0 \), and hence

\[ E^{(pz)}_A = 4\pi P^{(pz)}_A / \varepsilon_A. \]  

(3)

In the last case we implicitly assumed the cladding layer to be unstrained – that is, its lattice constant to be relaxed to its equilibrium value because its thickness exceeds the critical value for pseudomorphic growth over the substrate. \( P^{(pz)} \) may take any direction in general, but in normal practice its direction is parallel to the growth axis.\[ ]

To obtain piezoelectric polarization effects in zincblende semiconductor systems, lattice-mismatched epitaxial layers are purposely grown along a polar axis, e.g. (111); the in-plane strain propagates elastically onto the growth direction, thereby generating \( P^{(pz)} \). In wurtzite nitrides, the preferred growth direction is the polar (0001) [or (000\( \bar{1} \)] axis, so that any non-accommodated in-plane mismatch automatically generates a piezoelectric polarization along the growth axis (the sign depends on whether the epitaxial strain is compressive or tensile). We will be always be assuming this situation in the following.

Usually, alloys are employed in the fabrication of MQW’s. In that case, one may estimate the piezoelectric polarization in the spirit of Vegard’s law as, for a general strain imposed upon e.g. an Al\( _x \)Ga\( _{1-x} \)-N alloy,

\[ P^{(pz)} = \left[ x \varepsilon_{\text{AIN}} + (1-x) \varepsilon_{\text{GaN}} \right] \varepsilon(x), \]  

(4)

This expression contains terms linear as well as quadratic in \( x \), and similar relations hold for quaternary solutions. This piezoelectric term is only present in pseudomorphic strained growth, and will typically tend to zero beyond the critical thickness at which strain relaxation sets in. Uncomfortable though it may be, the Vegard hypothesis is at this point in time the only way we have to account for piezoelectric (and spontaneous, see below) fields in alloys. As will be shown below, indeed, the qualitative picture does not depend so much on the detailed value of the polarization field as on their order of magnitude.

III. SPONTANEOUS FIELDS IN MQW’S

New possibilities are opened by the use of III-V nitrides (AlN,GaN,InN), that naturally crystallize in the wurtzite structure. These materials are characterized by polarization properties that differ dramatically from those of the standard III-V compounds considered so far. From simple symmetry arguments[., it can be shown that wurtzite semiconductors are characterized by a non-zero polarization in their equilibrium (unstrained) geometry, named spontaneous polarization (or, occasionally, pyroelectric, with reference to its change with temperature)\[ ]

While the spontaneous polarization of ferroelectrics can be measured via an hysteresis cycle, in a wurtzite this cannot be done, since no hysteresis can take place in that structure. Indeed, spontaneous polarization has never been measured in wurtzites so far. III-V nitrides MQW’s offer the opportunity to reveal its existence and to actually measure it. In turn, spontaneous polarization can provide new degrees of freedom, in the form of permanent strain-independent built-in electrostatic fields, to tailor transport and optical characteristics of nitride nanostructures. Its presence can e.g. be exploited to cancel out...
the piezoelectric fields produced in typical pseudomorphically strained nitride structures, as discussed below.

Thanks to recent advances in the modern theory of polarization (a unified approach based on the Berry’s phase concept), it has become possible to compute easily and accurately from first principles the values of the spontaneous polarization, besides piezoelectric and dielectric constants, in III-V nitrides. The results of the calculations show that III-V nitrides have important polarization-related properties that set them apart from standard zincblende III-V semiconductors:

i) huge piezoelectric constants (much larger than, and opposite in sign to those of all other III-V’s);

ii) existence of a spontaneous polarization field of the same order of magnitude as in ferroelectrics.

The latter is, we think, a most relevant property. Spontaneous polarization implies that even in heterostructure systems where active and cladding layers are both lattice-matched to the substrate (so that no strain occurs, and hence no piezoelectricity), an electric field will nevertheless exist due to spontaneous polarization. In addition, unlike piezoelectric polarization, spontaneous polarization has a fixed direction in the crystal: in wurtzites it is the (0001) axis, which is (as mentioned previously) the growth direction of choice for nitrides epitaxy. Therefore the field resulting from spontaneous polarization will point along the growth direction, and this (a) maximizes spontaneous polarization effects in these systems, and (b) it renders the problem effectively one-dimensional. In the simplest case of a fully unstrained (substrate lattice-matched) MQW, the electric fields inside the layers are given, in analogy to Eq. (2) by

\[ E_A^{(sp)} = 4\pi \ell C (P_{C}^{(sp)} - P_A^{(sp)}) / (\ell C \varepsilon_A + \ell A \varepsilon_C) \]
\[ E_C^{(sp)} = 4\pi \ell A (P_A^{(sp)} - P_C^{(sp)}) / (\ell C \varepsilon_A + \ell A \varepsilon_C) \]  

(5)

where the superscript (sp) stands for spontaneous; typical spontaneous polarization values indicate that these fields are very large (up to several MV/cm).

In actual applications (for instance, to produce unstrained MQW’s) alloys will have to be employed. The values of the spontaneous polarization are accurately known only for binary compounds. In the absence of better estimates, we assume as before that the spontaneous polarization in alloys can be estimated using a Vegard-like rule (or C) layers of the MQW are lattice matched to GaN, which we assume to be also the substrate (or buffer) material (dashed-dotted line in Fig. 1). Then, piezoelectric polarization vanishes, but spontaneous polarization remains, and takes on values up to ~0.05 C/m². For a GaN quantum well with very thick AlGaN cladding layers, this means a theoretical electrostatic field of up to about 5 MV/cm.

IV. FIELDS IN THE GENERAL CASE

In general, of course, MQW’s will be strained. Then, for an arbitrary strain state, the electric fields in the A (or C) layers of the MQW are the sum of the piezoelectric and spontaneous contributions:

\[ E_{A,C} = E_{A,C}^{(sp)} + E_{A,C}^{(pz)} \]

where \( E_{A,C}^{(pz)} \) is the old-fashioned piezoelectric field from Eq. 3 and \( E_{A,C}^{(sp)} \) is given by Eq. 5. It is important to stress that \( E_{A,C}^{(sp)} \) depends only on material composition and not on the strain state. Also, it is a key point to notice that although both polarization contributions lay along the same direction [the (0001) axis], \( E_{A,C}^{(pz)} \) may have (due to its strain dependence) the same or the opposite sign with respect to the fixed \( E_{A,C}^{(sp)} \) depending on the epitaxial relations.
It is difficult to give a simple picture of the electric field pattern in a general MQW system because of the many degrees of freedom involved. Here we consider an Al$_x$Ga$_{1-x}$N/GaN MQW system (see text) vs. Al and In molar fraction. Fields are in units of MV/cm, positive fields point in the (0001) direction (Ga-face).

We now consider the field values in the active layer: the total field \( E \equiv -\nabla \phi \), in molar fraction. Fields are calculated for a given areal charge density (\( n_{2D} \)).

**Note again, at this point, that the fields (see Eqs. 2 and 3) are not related to just the polarization of the material composing the specific layer, but a combination of polarization differences, dielectric screening, and geometrical factors.**

We now consider the field values in the active layer: the total field \( E_A \) is shown in Fig. 2 vs. Al and In molar fraction; the same is done for the piezoelectric component in Fig. 3. In both cases the appropriate Vegard-like rules have been used.

Comparison of these Figures clearly bears out the importance of spontaneous polarization in determining the electric field. Several aspects are worth pointing out. First, large electric fields (~ 0.5–1 MV/cm), can be obtained already for modest Al and In concentrations. Second, it is easy to access compositions such that Al$_x$In$_y$Ga$_{1-x-y}$N is lattice matched to GaN; thereby, no piezoelectric fields exist, but large, purely spontaneous fields still do; specifically, this situation is realized for compositions laying on the zero-piezoelectric-field line in Fig. 2. Third, it is possible to choose the material composition in such a way that the active layers of a MQW’s are free of electric fields, despite the spontaneous polarization. To achieve this situation the MQW must be strained so that the piezoelectric and spontaneous polarizations cancel each other out; clearly, this is realized for compositions laying on the zero-field line in Fig. 2. Of course the possibility of having a null field where desired is of capital importance in those devices where electric fields in the active layer can not be tolerated (other field screening mechanisms are discussed below).

A noticeable feature of Fig. 3 is that the piezoelectric component increases much faster with In content that with Al content, despite the larger piezoelectric constants of the latter. The reason is, of course, that strain builds up much more rapidly with In concentration (in the Vegard hypothesis). On the other hand, it can be seen that the *spontaneous* component increases much more rapidly with Al content than with In content, due to the widely different polarizations of AlN and GaN.

**V. EFFECTS OF POLARIZATION FIELDS**

We now come to the implications of polarization fields for devices based on III-V nitrides. In this Section (with exception of Sec. IV), we present a set of accurate self-consistent tight-binding calculations for an isolated Al-GaN/GaN QWs representing a system in which the contribution to the total built-in electrostatic field of the spontaneous polarization is as large as the piezoelectric term. In realistic simulations of devices, self-consistency is needed to describe field screening by free carriers; the latter cannot physically cancel out the polarization charge, which is fixed and invariable, but may screen it out in part. In our calculations we therefore solve self-consistently the Poisson equation and the Schrödinger equation for a state-of-the-art empirical tight binding Hamiltonian for realistic nanostructures. In the following two cases are considered: (a) non-equilibrium carrier distribution (Sec. A and B) related to photoexcitation or injection, where electron and hole quasi-Fermi levels are calculated for a given areal charge density \( n_{2D} \) in the quantum well (the sheet density, related to the injection current or optical pumping power); (b) thermal
equilibrium distribution (Sec. D) where the Fermi level is calculated as a function of doping density by imposing charge neutrality conditions. We solve Poisson’s equation,

\[
\frac{d}{dz}D = \frac{d}{dz} \left( -\varepsilon \frac{d}{dz}V + P_T \right) = \varepsilon (p - n),
\]

where the (position-dependent) quantities \(D\), \(\varepsilon\), and \(V\), are respectively the displacement field, dielectric constant, and potential. \(P_T\) is the (position-dependent) total transverse polarization. The effects of composition, polarization, and free carrier screening are thus included in full. Consistently with the aim of describing a single QW, we choose the boundary conditions of zero field at the ends of the simulation region.

The potential thus obtained is inserted in the Schrödinger equation, which is solved diagonalizing the empirical tight-binding \(sp^3d^5s^*\) Hamiltonian. The procedure is iterated to self-consistency. Further applications and details on the technique can be found elsewhere.

Here we concentrate in particular on the polarization-induced quantum-confined Stark effect (QCSE) in zero external field, and its control and quenching. We first deal with the low free-carrier densities regime: thereby the QCSE manifests itself as a strong red shift of the interband transition energy, with a concurrent suppression of the transition probability, both of these features getting stronger as the well thickness increases. This is the regime that applies to low-power operation or photoluminescence experiments.

Next we discuss how the QCSE can be modified, and eventually (almost) quenched, by providing the QW with a sufficiently high free-carrier density. In this regime, as the free carrier density increases, the transition energy is progressively blue-shifted back towards its flat band value, and the transition probability suppression is largely removed. The needed free-carrier density depends on the polarization field, and not surprisingly it is found to be typically very substantial. Typical values of the sheet density range in the 10^{12} cm^{-2}, as opposed to typical values of 10^{11} cm^{-2} needed to obtain lasing in GaAs-like materials.

### A. QCSE at low power

The prototypical system we consider is an isolated GaN quantum well cladded between Al_{x}Ga_{1-x}N barriers. In Fig. 4, similarly to Fig. 3, we display the total field \(E_A\) in the (isolated) active well, and its piezoelectric component as a function of the Al molar fraction \(x\). The spontaneous component is the difference of the two, and therefore approximately equal to the piezoelectric one.

The value we pick for our simulations is \(x=0.2\), a reasonable compromise between the conflicting needs for not-too-large fields, sufficient confinement, and technologically achievable composition. In this case the valence offset is \(\Delta E_v = 0.064\) eV. The total field in the QW of \(-2.26\) MV/cm, and the spontaneous and piezoelectric components are \(-1.14\) MV/cm and \(-1.12\) MV/cm respectively. The minus signs indicates that the field points in the (001) direction. The bare polarization charge at the interface is proportional to the change in polarization across the interfaces, and it amounts to \(\sim 1.28 \times 10^{13}\) cm^{-2}. The field value mentioned above results from this charge as screened by the dielectric response of the QW (the field change at the interface is thus related to a smaller, or screened, effective interface charge).

![FIG. 4. Total field and its piezoelectric component in the GaN/Al_{x}Ga_{1-x}N QW discussed in the text.](image)

We have performed a series of calculation for different well width where the electron and hole confined states have been populated (i.e. pairs have been created) with a density of \(\sim 10^{11}\) cm^{-2} to simulate a low-power optical excitation. We find that this density has only a very marginal effect: indeed, the potential is perfectly linear, i.e. the electrostatic field remains uniform, over essentially all the QW. The square-to-triangular change in the potential shape causes a small blue shift of both the electron and hole confined states (referred to the flat well bottom), but the linear potential given by the field causes a much larger relative red shift for any reasonable thickness. Also, since the thermal carrier density fluctuations are negligible at microscopic thicknesses and room temperature (see below and Ref. 16), one expects the QW band edge profile to remain linear as function of thickness, at least for the low excitation powers typical of photoluminescence spectroscopy.

In Figure 5 we show the TB result for the lowest interband transition energy and the corresponding transition probability (i.e. the squared overlap of the highest
hole level and the lowest electron level envelope wavefunctions as a function of QW thickness. Both the Stark red shift and the strong suppression of the transition probability are evident, as was to be expected from the potential shape and the reduced overlap of hole and electron states (see inset Fig. 5).

It is worth noting that the localization of the hole envelope function in the well region is rather weak, because the large effective field blue-shifts the hole bound state energy close to the valence barrier edge. This will generally be the case for low-$x$ AlGaN wells, due to the small valence confinement energy.

In fact, on the scale of the fields-induced potential drop, even the conduction confinement is small, and the electron bound state also tends to have the character of a resonance for small $x$ (i.e. small confinement).

We conclude that in the absence of excitation and at normal operation temperatures, or at low optical excitation powers, macroscopic polarization fields cause QW’s to be highly inefficient in emitting light, and the emission energy to be considerably different than the gap of the material plus confinement energies.

Comparison with experiment is tricky since most attempts to measure these effects are polluted by (typically unnecessary) complicated choices of the geometry. In any case, the general experimental features are in full agreement with the notion that the transitions are red-shifted essentially linearly with increasing well thickness, and that screening at low free carrier densities is irrelevant in this class of systems. This is not quite true any more for thick layers, as will be discussed in Sec. V C.

B. QCSE quenching at high excitation power

If carriers are generated optically, one can envisage that a sufficiently high excitation power could possibly produce the carrier density needed to screen the polarization field. We now calculate the properties of the QW as a function of the free-carrier areal density, to check if the red shift and the transition probability suppression can be removed in a physically accessible range of such density.

We repeat the self-consistent procedure increasing progressively the free charge density in the QW, from $10^{12}$ up to $2 \times 10^{13}$ cm$^{-2}$. We see in Fig. 6 that, albeit at the cost of a large increase of the QW free-carrier density, the field does get progressively screened.

As can be seen in Fig. 7, at fixed thickness the red shift decreases as a function of carrier density, and it tends to become thickness-independent at the highest densities. The transition probability is also increased by several orders of magnitude; however, the field is not screened abruptly but dies off gradually, with an effective screening length of about 20 Å for the largest density used here (of course, this is a token of the larger spatial extension...
of the screening charge as compared to the polarization charge. Therefore, holes and electron remain spatially separated to a large extent even at high carrier densities, and the transition probability never quite goes back to unity. This is not unlikely to be one of the reasons for the relatively low quantum efficiency observed in typical nitride MQW devices. For the same reasons, the transition energy never goes back exactly to the flat-band value (gap plus confinement energy). Note in passing that because of strain, in these calculations \(E_g^{\text{GaN}} = 3.71\) eV, almost 10% larger than the equilibrium value.

Another noticeable effect is that at a properly chosen value of the sheet density (i.e. of the excitation power) one can obtain at the same time a reasonable transition probability and a red-shifted energy by just increasing the well thickness. This is very useful since the transition wavelength can be shifted to a different color without changing alloy composition, but only the well thickness. For instance (see Fig. 7), changing the well thickness from 20 to 30\(\,\text{Å}\) at a sheet density of \(4 \times 10^{12}\,\text{cm}^{-2}\), one obtains an energy shift of 0.1 eV at the cost of a loss of a factor 10 in recombination rate, which may still be acceptable depending on the application. Red-shifting the transition energy in this fashion may avoid the need to add e.g. some In in the QW composition.

C. Screening of fields in massive samples

Free charge produced by high excitation power adsorb radiation at many different transition energies ranging from that of the built-in field–biased well (low power limit) to the quasi–flat-band well (high power limit) – that is, the MQW is a multistable switch. It is indeed fortunate that the typical fields in these structures are such that one can physically access the various possible regimes.

The screening density of order \(2 \times 10^{13}\,\text{cm}^{-2}\) needed to partially screen out the field corresponds to an optical pumping power of about 10 to 20 kW/cm\(^2\) per well, as can be estimated from Refs. [18–20]. This figure agrees nicely with the unusually high pumping powers[2] needed to obtain the laser effect in nitride structures. The explanation is simply that much of the free charge being generated actually goes into screening the polarization field. On the other hand, our result prove that the optically activated lasing conditions can indeed be realized in practice, although with high pumping powers, since these seems to be no need to invoke quantum dot formation[13] or other exotic effects to explain lasing in nitride structures. On the other hand, the same phenomenon explains the high current threshold observed for electrically driven GaN based lasers.[21–23]

QCSE quenching phenomena similar to those just described have been observed by Takeuchi et al.[13] in InGaN wells, with estimated fields in the 1 MV/cm range. The red shift and optical inefficiency can in fact be removed, although only in a transient fashion, by sufficiently high excitation powers. The order of magnitude of the values reported in Ref. [13] is \(~200\,\text{kW/cm}^2\) for 5 to 10 MQW periods, i.e. 20 to 40 kW/cm\(^2\) per well, in qualitative agreement with our estimate above. One important remark at this point is that, depending on the excitation power, the MQW will adsorb radiation at many different transition energies ranging from that of the built-in field–biased well (low power limit) to the quasi–flat-band well (high power limit) – that is, the MQW is a multistable switch. It is indeed fortunate that the typical fields in these structures are such that one can physically access the various possible regimes.

![FIG. 7. Removal of red shift and recovery of interband transition probability upon high excitation.](image)

For this picture to hold, the spatial extension of the screening charge at the sample surface must be comparable with that of the polarization charge (which is a few
Indeed decreases progressively as for the thicker wells, the field (while remaining uniform) consistent TB results.

A first point to note is that the field remains uniform effective masses in this model where fitted with the TB model in order to reproduce quite accurately the self-constituent TB results.

The resulting self-consistent potential is shown in Fig. for well thicknesses of 100, 200, 300, and 400 Å lengths. A first point to note is that the field remains uniform for all well thicknesses. The field value equals the polarization field for the smallest thickness (smaller than $d_c$); for the thicker wells, the field (while remaining uniform) indeed decreases progressively as $\propto 1/d$.

$$E \propto \frac{1}{d}$$ and much smaller that the sample size. This will cause the field inside the sample to remain uniform, since the net effect of screening will be to change the effective polarization charge. In fact, this assumption turns out to be verified in practice on direct inspection, as we discuss below.

Clearly, the above mechanism will strongly influence QW’s of thicknesses equal to, or larger than, the critical value $d_c$. For the QW we are considering here, with a polarization field of $-2.26$ MV/cm, the critical value is $d_c \sim 165\,\text{Å}$. To confirm our picture, we simulated QW’s with the same composition and geometry considered in Sec. B, and thicknesses below and above $d_c$, to mimic the crossover from a “microscopic” to a “macroscopic” sample. In this case, we need to describe very extended bulk regions on the left and right of the QW, in order to account for the large screening length. Thus, we have made use of a classical Thomas-Fermi model where the charge densities are calculated with Fermi-Dirac statistics of a classical system rather than by solving the Schrödinger equation in the TB basis. This allows to consider devices with a spatial extension of several hundreds of microns. Effective masses in this model where fitted with the TB model in order to reproduce quite accurately the self-consistent TB results.

The resulting self-consistent potential is shown in Fig. for well thicknesses of 100, 200, 300, and 400 Å lengths. A first point to note is that the field remains uniform for all well thicknesses. The field value equals the polarization field for the smallest thickness (smaller than $d_c$); for the thicker wells, the field (while remaining uniform) indeed decreases progressively as $\propto 1/d$.

Photoluminescence experiments are not expected to be able to reveal this effect (which should cause a saturation of the red shift as function of thickness) in very thick QW’s, since the effective recombination rate is vanishingly small at the relevant thicknesses. Experiments aiming to reveal this effect should be designed considering our results that a very thick layer is effectively subjected to a uniform electrostatic field $E_{\text{gap}}/d$. In an unstrained GaN QW, for $d > d_c$, (the latter being typically of order a few hundred Å or so depending on the polarization) the field is $\sim 3.4 \,\text{V/cm}$, i.e. $\sim 70 \,\text{kV/cm}$ for $d = 0.5 \,\text{µm}$. This is presumably sufficient to cause observable bulk-like effects such as shifts in response functions or field effects on impurities.

A similar “self-screening” behavior has been revealed indirectly in devices comprising sufficiently thick layers. In Ref. a 300 Å thick Al$_{0.15}$Ga$_{0.85}$N layer was grown on a very thick GaN substrate, and topped with a Schottky contact. The predicted field in the AlGaN layer is $1.4 \,\text{MV/cm}$, which would cause across the layer a potential drop of $4.2 \,\text{eV}$. The maximum reasonable potential drop dictated by Schottky barriers, conduction offset, and Fermi level is about 1 eV, so it must be the case that the polarization charge gets largely screened by electrons from the GaN layer, forming a high-density two-dimensional electron gas (2DEG) at the heterointerface; this, by the way, causes an enhanced mobility in the conducting channel. CV depth profiling indeed reveals a 2DEG at the interface. An equivalent, more formal description is: the field, if assumed uniform, would force the metal-determined Fermi level to some 3 eV above the conduction band of GaN, thus attracting towards the interface an enormous carrier density, which screen (part of) the field out. Note in passing that in Ref. only piezoelectric polarization was considered, which leads to an underestimation of the 2DEG density, since the piezoelectric contribution is actually about one third of the total interface charge. Similar considerations apply to other similar recent experiments. A recent device simulation has corrected this point, including in part the spontaneous-polarization interface charges.

D. Suppressing QCSE by doping

We have seen in the previous Sections that polarization fields can be screened to a reasonable extent by generation of free charge of both kinds in the QW upon e.g. optical excitation. Qualitative problems with this screening mechanism are that (a) it is transient, since it disappears when photoexcitation or current injection are removed, and that (b) in purely electronic (i.e. non-optoelectronic) devices, it is unlikely that the high densities needed can be reached in normal operating conditions. Besides, the injected current is not constant in time, so that the well shape changes in time.

It is natural to presume that the same effects can be achieved in a permanent fashion using extrinsic carriers from dopants. The idea is to provide the well with carriers which would screen the polarization charge, excepts that now the electrons are released into the QW from
the doped barriers, and not injected or photogenerated. Of course, this effect is not transient as the others discussed previously. The problem is, how high must the doping density be to achieve the same level of screening as in a high optical excitation regime. We simulated a 50 Å thick Al$_{0.2}$Ga$_{0.8}$N/GaN single QW, where the barriers have been doped n-type in the range from $10^{17}$ to $10^{20}$ cm$^{-3}$ and the donor ionization energy have been set to 10 meV. We used in this simulation a selfconsistent TB approach. The resulting conduction band profile is displayed in Figure 9 for the various doping densities.

![Figure 9](image-url)

**FIG. 9.** Selfconsistent conduction band edge of a remotely doped well.

The polarization field raises the conduction band on the left side over the Fermi energy and in order for the barrier conduction band to reach the Fermi level on the far left, the electrons are transferred from the left-side barrier into the QW, leaving behind a large depletion layer. As a consequence of the electron flow into the QW, the polarization field start to get significantly screened at doping densities above $\sim 10^{19}$ cm$^{-3}$. The existence of a depletion layer causes a large band bending in the barrier, while the bending is absent in the left half of the well. This is quite different to the case of the photoexcited well, where the bending on the left side of the well was due to hole accumulation nearby the interface (see Fig. 6). This explains why the field remains nearly uniform in the left half of the well for all of the simulations performed. On the right side of the well only a small bending due to the electron accumulation is present. Indeed electron localization is quite weak in these systems since the confinement potential is small as compared to the field-induced drop, and electrons tend to spill over to the right-side barrier. This is likely to be case in all nitride systems in this composition range.

From these results, we conclude that doping can indeed be used to screen polarization fields. While it is not obvious that the needed doping level can always be reached in practice, it is likely that a combination of doping and current injection or photoexcitation will generally succeed in quenching the polarization field in the range of MV/cm recovering a quasi flat band condition. Fields in InGaN/GaN systems will be generally smaller than those in AlGaN/GaN systems for typical compositions in use today, and will therefore be more easily amenable to treatment by the above technique. This procedure has in fact been adopted in experiment by Nakamura’s group [4] which reported that a doping level of $10^{19}$ cm$^{-3}$ is sufficient to quench the QCSE to a large extent. Indeed in their In$_{0.15}$Ga$_{0.85}$N/GaN MQW’s the unscreened field is $\sim 1.2$ MV/cm, i.e. approximately a half of the one we considered here thus easily screened by remote doping, this conclusion is in qualitative agreement with our findings.

**VI. SUMMARY AND ACKNOWLEDGEMENTS**

In conclusion, we have discussed how macroscopic (and in particular, spontaneous) polarization plays an important role in nitride-based MQW’s by producing large built-in electric fields. Contrary to zincblende semiconductors, in III-V nitrides–based devices the spontaneous polarization is an unavoidable source of large electric fields even in lattice-matched (unstrained) systems. The existence of these fields may also be used as additional degree of freedom in device design: for instance, for an appropriate choice of alloy composition, spontaneous and piezoelectric fields may be caused to cancel out, thus freeing the structures from built-in fields. We have also discussed the different regimes of free carrier screening, affected by doping or optical excitation, showing that fields can be screened only in the presence of high free carrier densities, which leads to unusually high lasing thresholds for undoped QW’s. Of course, our results about the effects on the electronic structure apply qualitatively to any kind of polarization field, thus in particular also to piezo-generated ones.

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From dielectric displacement conservation (see Ref. [2]) one gets \(4\pi(P_C - P_A) = \varepsilon_A E_A - \varepsilon_C E_C\). Periodicity implies \(\ell_A E_A + \ell_C E_C = 0\). Solving for one of the fields, Eqs. [3] are immediately obtained.

This assumption is valid in the limit in which the electric field across the whole structure is negligible with respect to the internal fields induced by polarization. This is verified e.g. when the MQW system is embedded on both sides by doped materials of the same composition.

Note that for normal devices layered along the nominal growth direction, the electric field is always parallel to the growth direction, even if the polarization is not.

Vegard-like estimates of the polarization should of course be considered with caution, as it is established (see e.g. P. Ernst, C. Geng, M. Burkard, F. Scholz, and H. Schwizer, in The Physics of Semiconductors, M. Scheffler and R. Zimmermann eds. (World Scientific, 1996), p. 469; S. Froyen, A. Zunger, and A. Mascarenhas, Appl. Phys. Lett. 68, 2852 (1996)) that ordering in (cubic) III-V solid solutions can produce spontaneous polarization, an effect not unexpected also in the XN’s. Even in the random solution, short-range order in the form of bond alternation may alter the local electronic structure, hence the polarization.

One possible way to see it is as the zero-strain limit of the piezoelectric polarization.

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