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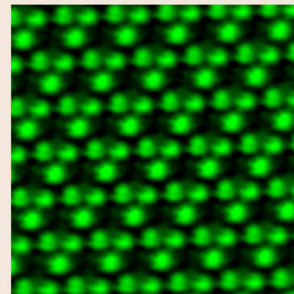

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Doping screening of polarization fields in nitride heterostructures

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Using self-consistent tight-binding calculations, we show that modulation doping can be used to screen macroscopic polarization fields in nitride quantum wells. The blue-shift of photoluminescence peak as well as the reduction of radiative recombination lifetime at increasing doping density is explained and correlated to polarization-field screening. The field-induced ionization of the dopants and its relation with alloy composition in the heterostructure barriers is also analyzed. © *2000 American Institute of Physics.* [S0003-6951(00)05026-9]

Laser structures based on III–V nitride multiquantum wells (MQWs) have been shown to benefit from doping of the active region.[1] However, several puzzles remain concerning the mechanisms involved. Experimentally, it has been established for both GaN/InGaN[2–9] and AlGaN/GaN[10–12] heterostructures that doping of the active region produces (i) a blue-shift of the photoluminescence (PL) peak, (ii) an enhancement of the emission intensity, (iii) a reduction of the laser threshold current, (iv) a reduction of the carrier radiative recombination lifetime, and (v) a reduction of the Stokes shift between PL peak and the photoluminescence excitation (PLE) spectra. Based on phenomenological arguments, it has been suggested that the observed phenomena is due to (a) doping-enhanced growth quality of the active region,[3,4,8,11,13] (b) doping screening of polarization fields,[3,5,6,9] or (c) screening of potential fluctuations.[4–6,8]

Despite its relevance to laser design, the doping effect has been only marginally touched upon theoretically.[9,14] In this letter we apply the self-consistent procedure outlined in Refs. 14–16 to AlGaN/GaN and GaN/InGaN MQW systems, investigating how piezoelectric and spontaneous[14,17–19] polarization fields can be screened via n- and p-type doping. Further, we consider the screening interplay of extrinsic and injected carriers, experimentally investigated in Ref. 6.

We solve the Schrödinger equation in the nearest-neighbor $sp^3d^5s^*$ tight-binding (TB) basis,[20] self-consistently coupled with a one-dimensional (1D) Poisson equation accounting for polarization, doping, and free carriers.[14–16] The macroscopic polarization in the alloys are obtained by Vegard interpolation of *ab initio* values[17] for the binary compounds. This procedure describes the interplay of polarization and dielectric, free-carrier, and doping screening in a fully self-consistent and nonperturbative way, with band structure accuracies typical of *ab initio* methods.[20] Optical properties are obtained via the Graf–Vogl theory[21] without introducing additional fitting parameters. The method has been previously employed to describe wide-gap MQW and interface systems.[14,15,19,22]

We performed calculations at room temperature for $Al_{0.15}Ga_{0.85}N/GaN$ and $In_{0.2}Ga_{0.8}N/GaN$ MQWs, with 100 Å barriers and 40 Å wells, pseudomophically grown on a GaN substrate. We considered purposely modulation-doped (doped barrier) structures, assuming a $10^{17}\,cm^{-3}$ residual doping in the wells. The extrinsic levels are chosen among a 20 meV bound donor, and shallow (20 meV) or deep (250 meV) acceptors, the "deep" level representing typical p-dopants in GaN.[23]

The results for the AlGaN/GaN MQWs are shown in Fig. 1. The optical gap [the separation between the first quantized conduction (C1) and valence (V1) levels] and the C1–V1 oscillator strength (proportional to the C1–V1 radiative transition probability) are plotted respectively in Figs. 1(a) and 1(b) as a function of the doping density, for several values of an externally injected free carrier density (n_{2D}). Inclusion of the latter allows us to mimic lasing under electrical or optical pumping.

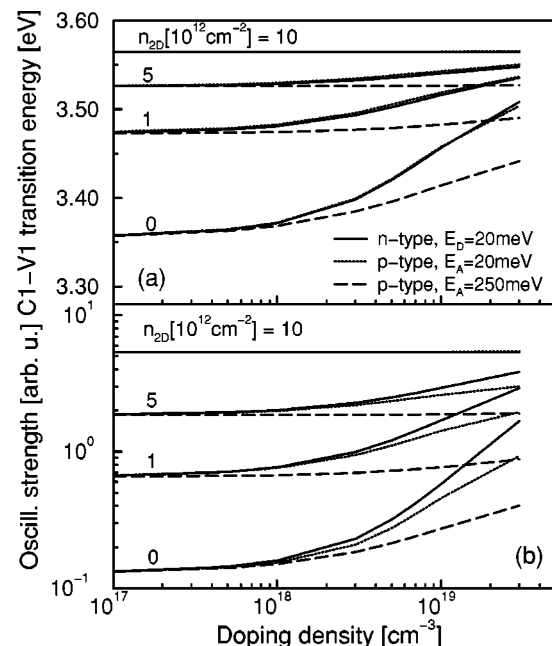

FIG. 1. Ground-level-emission transition energy (a) and oscillator strength (b) in $Al_{0.15}Ga_{0.85}N/GaN$ MQWs, as a function of p or n doping densities, at different values of free-charge injection.

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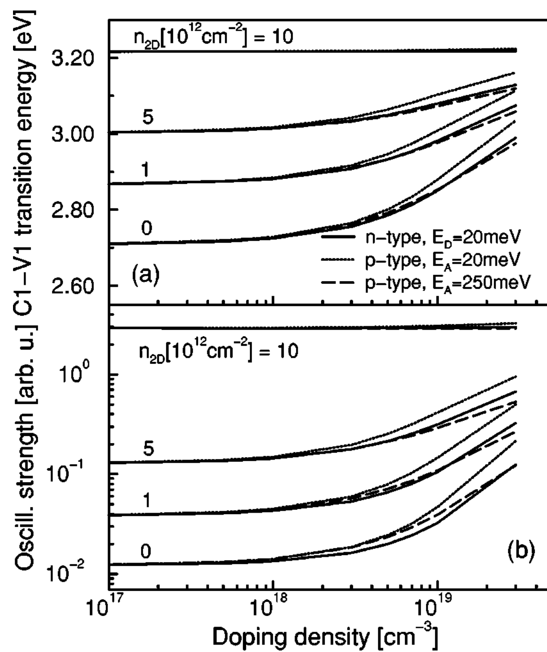

FIG. 2. As in Fig. 1, for $GaN/In_{0.2}Ga_{0.8}N$ MQWs.

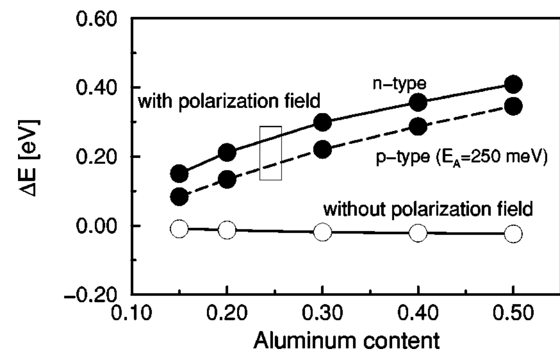

FIG. 3. Shift of the C1–V1 transition vs x in $Al_xGa_{1-x}N/GaN$ MQWs, calculated as the difference of the C1–V1 transitions for doping levels of 3×10^{19} and $10^{17}\,cm^{-3}$.

At zero injection ($n_{2D}=0$), the extrinsic carriers from ionized dopants partially screen the macroscopic polarization field. For both n- and shallow p-doping, the fundamental transition energy blue-shifts by as much as 150 meV when the doping density is increased from 10^{17} to $3\times10^{19}\,cm^{-3}$). Deep (i.e., the actual) acceptors are much less efficient in screening the polarization and cause a blue-shift of only 80 meV. Indeed, larger dopant binding energy implies fewer ionized centers, hence fewer free carriers in the well. Upon free-carrier injection, the doping-induced blue-shift is reduced. This is expected since screening is already activated by the injected free charge itself (notably at high injection).

The radiative probability of the C1–V1 transition [Fig. 1(b)] is related to the laser threshold current. In the absence of carrier injection, the transition probability increases by an order of magnitude in going from low to high doping densities. In fact, doping screening of the field increases the overlap between confined conduction and valence states, enhancing the radiative transition probability. We found that the increase in transition probability is lower for shallow p doping than for n doping. This result depends on the different density of states and band offsets for electron and holes.

For laser operation, however, the case with injected carriers is more relevant. As for the transition energy, the higher the injected density, the smaller the doping-induced shift: at high injection, the polarization field is already screened even for low doping. However, for typical laser-operation densities, a moderately high doping does increase the transition probability. For $10^{19}\,cm^{-3}$ doping, one obtains the the same recombination probability at injection $n_{2D}=5\times10^{12}\,cm^{-2}$ as at $n_{2D}=10^{13}\,cm^{-2}$ with no doping. Since the recombination probability is inversely proportional to the spontaneous recombination lifetime, the laser threshold current will be reduced by proper doping design.

The doping dependence of transition energies and probability in GaN/InGaN MQWs is shown in Figs. 2(a) and 2(b), respectively. The overall effect of doping is stronger than in the AlGaN/GaN case, the blue-shift amounting to 280 meV for n doping and for deep-level p doping, and up to 325 meV for shallow-level p doping. The higher efficiency of doping screening in GaN/InGaN wells is due to polarization field being larger than in AlGaN/GaN ones (the polarization charge is $0.03\,C/m^2$ at $GaN/In_{0.2}Ga_{0.8}N$ interfaces, compared to $0.013\,C/m^2$ at $Al_{0.15}Ga_{0.85}N/GaN$ ones). The field-induced ionization (FII) of the dopant (already pointed out in Ref. 24) is consequently larger in the GaN/InGaN than the in AlGaN/GaN structure. The FII effect is also responsible for the comparable effectiveness of the deep p and n-type doping. Under high injection condition, the same trends are observed as in the AlGaN/GaN case.

The degree of field ionization of the dopants in the barriers depends on the barrier material, via the alloy composition dependence of polarization fields. Hence, the screening efficiency should depend on composition. Indeed, consider Fig. 3, displaying the C1–V1 transition blue-shift obtained by raising the doping density from 10^{17} to $3\times10^{19}\,cm^{-3}$, as a function of Al concentration in the AlGaN barrier, and considering both n and deep p doping. The increased Al content enhances the electric field in the structure, hence the ionized dopant density: consequently the blue-shift is larger at large Al concentrations. Again, the deeper level screens less efficiently.

Neglect of polarization yields, as expected, a shift which is negligible on the relevant energy scale. This does not necessarily imply that the *density* of ionized impurities is reduced when polarization fields are neglected. While this is the case for p doping because of the acceptor depth,[24] it is not for n doping, where the percentage of ionized dopants with and without polarization fields are comparable. As Fig. 4 shows, the key effect of the field is to ionize the impurities *asymmetrically*. The ionized (positive) centers and the electrons transferred into the well form a dipole which screens the field. If the field is zero, the ionization will be symmetric with respect to the quantum well, and no dipole will result.

In conclusion, we have shown that doping induces a blue-shift of the optical transition, larger for low injected carrier density. Doping increases the transition probability at the optical gap. This explains the experimental findings of lower laser threshold current, reduced radiative lifetime, and increased emission intensity in doped MQWs. Because of field ionization of the dopants, the doping screening efficiency depends on heterostructure composition. All free-

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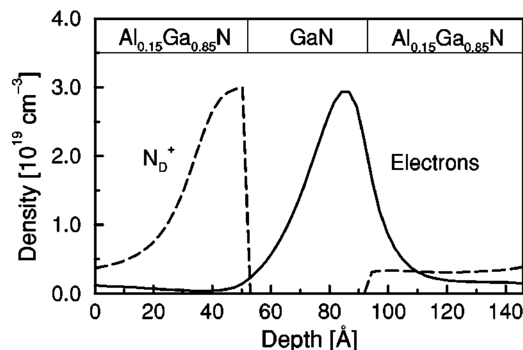

FIG. 4. Ionized dopant density (dashed lines) and electron density (solid line) in a *n*-doped (3×10^{19} cm^{-3}) $Al_{0.15}Ga_{0.85}N$/GaN MQW.

charge related values (such as blue-shifts, PL intensity, Stokes-shifts, etc.) will thus depend both on doping and material composition. We conclude that doping is an additional degree of freedom to tune nitride lasers for efficiency.

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