

Internal electric-field and segregation effects on luminescence properties of quantum wells

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Surface segregation of In atoms during molecular-beam epitaxy and its influence on the energy levels in strained piezoelectric InGaAs/GaAs and InGaN/GaN quantum wells (QWs) are investigated theoretically. It is shown that these effects modify the electronic states in the QW and the emission energy in the photoluminescence (PL) spectra. In this work, we solve analytically the Schrödinger equation in the absence of electric field, taking into account the shape changes in the QWs due to the segregation of In atoms during the growth process of the semiconductor heterostructures. Furthermore, the influence of the built-in electric field due to the piezoelectric effect on the PL emission is calculated by considering a variational electron wave function to calculate the ground-energy transitions inside the active region in the heterostructure. In particular, we apply this model to the case of indium segregation in InGaAs/GaAs for moderate internal electric fields. The transition energy calculations between the confined electron and hole states as a function of the well width for different temperatures and In composition are in agreement with the measured PL energy peaks. © 2005 American Institute of Physics. [DOI: 10.1063/1.1954889]

I. INTRODUCTION

GaN-based quantum wells (QW's) attracted much interest in the last few years since they have become the key material in commercial fabrication of long-time light-emitting diodes (LED's) and laser diodes for the blue to ultraviolet spectral range. Up to now InGaN/GaN is used as an active region in these devices. However, the light-emitting mechanism is not yet full understood because this material exhibits some peculiarities.

The rather poor structural material quality in terms of defect density, compositional homogeneity, abrupt interfaces, etc., compared to other heterostructures is mainly a consequence of a strong chemical difference between GaN and InN. It results, e.g., from a large mismatch between well and barrier material associated with a high dislocation density. Much effort has been made to investigate the spatial extension and depth of composition fluctuations as well as their impact on the optical properties.¹

Another peculiarity results from the polar axis of the wurtzite crystal structure and the strong polarity of III-N bindings. All group-III nitrides in the wurtzite phase have a strong spontaneous macroscopic polarization and large piezoelectric coefficients. This has been found from *ab initio* calculations.^{2,3} The abrupt variation of the polarization at the surfaces and interfaces gives rise to large polarization sheet charges that in turn create internal electric fields of the order of MV/cm. The field-induced linear bending of the band edges causes a spatial separation of confined electrons and holes within the active layers of the devices and has, there-

fore, important consequences on the optical properties of the nitride-based light-emitting diodes or lasers. It is worth noting that the piezoelectric field present in the III-V nitrides appears in the presence of strain, due to, e.g., epitaxy, while the spontaneous polarization is a property of low-symmetry materials in their ground state, independent of strain, and it is absent in zinc-blende materials (e.g., GaAs). The InGaAs/GaAs system is the typical pseudomorphic heterostructure in which moderate electric fields can be produced. Recently,⁴ the pseudomorphic In_xGa_{1-x}As/GaAs QW's were grown by molecular-beam epitaxy on GaAs substrates oriented along (11*n*) directions, with *n*=1, 2, 3, and 4, where the optical and structural properties of the devices were studied by photoluminescence (PL), photoreflectance spectroscopy, and atomic force microscopy measurements.

Furthermore, besides the built-in electric field, a strong tendency of indium surface segregation during the growth of InGaAs/GaAs and InGaN/GaN QW's result in nonabrupt interfaces and surface compositions different from the bulk. Segregation is the process whereby binding- and elastic energy differences between surface and bulk sites result in the migration to the surface of one species. The heteroepitaxy of InGaAs (InGaN) layer on GaAs (GaN) substrates is characterized by a strong segregation of indium atoms that accumulate at the growth front and substantially modifies the In-composition profile, resulting in different electronic and optical properties of the devices based on that materials. For different segregation lengths corresponding to different growth temperature ranges, the potential profile has been calculated using the segregation equations proposed by Muraki *et al.*⁵ Their phenomenological model has been show to de-

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