Applied Surface Science 166 (2000) 300–303
applied surface science
www.elsevier.nl/locate/apsusc

Misfit dislocations and radiative efficiency of $In_xGa_{1-x}N/GaN$ quantum wells

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Abstract

We report results of calculations of radiative efficiency of $In_xGa_{1-x}N$ quantum wells embedded in wurtzite GaN epilayer. It was found that misfit dislocations with density up to $\sim 10^{5-6}$ cm^{-1} could improve the quantum efficiency of the $In_xGa_{1-x}N$ wells by more than 10 times because they reduce the quantum well built-in electric field. At higher densities, the misfit dislocations suppress the quantum efficiency of the wells since they produce an additional channel of nonradiative recombination.

PACS: 73.20.Dx
Keywords: GaN; Quantum well; Quantum efficiency; Dislocations; Built-in electric field

The most common defects in wurtzite GaN epilayers grown on sapphire are threading dislocations originating from high-lattice mismatch between the epilayer and substrate [1]. These defects can significantly affect the nonequilibrium carrier lifetime at low injection levels and prevent low laser thresholds [2,3]. Recently, dislocations of another type, localized in the $In_xGa_{1-x}N$ quantum wells, have been observed, which most probably are the misfit dislocations at $GaN/In_xGa_{1-x}N$ interface [4].

In the present paper, we investigate the influence of the misfit dislocations at the interface of the $In_xGa_{1-x}N$ quantum well on the radiative efficiency of the carriers in quantum wells. This influence arises from two factors. First, the dislocations act as nonradiative recombination centers and reduce the quantum efficiency. Second, the misfit dislocations partially release the strain inside the well and suppress the built-in electric field. This leads to an increase in the optical matrix element for the electron-hole radiative recombination in the well and improves the quantum efficiency. Thus, for finding out the effect of the misfit dislocations on the quantum efficiency of light-emitting devices, both above factors should be taken into account and analyzed simultaneously.

The built-in electric field in the well, $E^{\rm in}$, arises from piezoelectric polarization, $P^{\rm in}_{\rm PE}$, the spontaneous polarization, $P^{\rm in}_{\rm SP}$, and the electric induction outside the well, $D^{\rm out}$, and is given by the equation

$$E^{\rm in} = \frac{D^{\rm out} - P^{\rm in}_{\rm PE} - P^{\rm in}_{\rm SP}}{\varepsilon\varepsilon_0} \qquad (1)$$

where ε and ε_0 are the dielectric constants of the material and vacuum, respectively.

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0169-4332/00/$ - see front matter
PII: S0169-4332(00)00437-2

The electric induction outside the well is given by

$$D^{\text{out}} = \varepsilon\varepsilon_0 E^{\text{out}} + P^{\text{out}}_{\text{PE}} + P^{\text{out}}_{\text{SP}} \tag{2}$$

where E^{out}, $P^{\text{out}}_{\text{PE}}$ and $P^{\text{out}}_{\text{SP}}$ are the electric field, piezoelectric polarization and the spontaneous polarization outside the well, respectively.

For the epilayer with unstrained barriers which are considered below, the piezoelectric polarization in the barriers is zero, $P^{\text{out}}_{\text{PE}} = 0$. If the barrier thickness, d_{B}, is wider than the spontaneous ionization thickness, $d_0 = \varepsilon\varepsilon_0 E_{\text{g}} / eP^{\text{out}}_{\text{SP}}$ ($d_0 = 100$ Å for GaN), the electric field E^{out} in the barriers is negligibly small, $E^{\text{out}} < d_0 P^{\text{out}}_{\text{SP}}$, and we get the following equation for the electric field E_{in} inside the well in the case $d_{\text{B}} \gg d_0$

$$E^{\text{in}} = \frac{P^{\text{out}}_{\text{SP}} - P^{\text{in}}_{\text{PE}} - P^{\text{in}}_{\text{SP}}}{\varepsilon\varepsilon_0} \tag{3}$$

where

$$P^{\text{in}}_{\text{PE}} = 2\left(\frac{a_{\text{out}}}{a_{\text{in}}} + a_{\text{in}} N^{\text{misfit}}_{\text{d}} - 1\right)\left(e^{\text{in}}_{31} - e^{\text{in}}_{33}\frac{c^{\text{in}}_{13}}{c^{\text{in}}_{33}}\right) \tag{4}$$

and $a_{\text{in (out)}}$ are the lattice constants inside (outside) the well; e^{in}_{ik} and c^{in}_{ik} are the piezoelectic coefficients and the elastic constants in the well, respectively; $N^{\text{misfit}}_{\text{d}}$ is the density of the misfit dislocations per unit length at the well interface.

The dependence of the built-in electric field inside the $\text{In}_x\text{Ga}_{1-x}\text{N}$ well embedded in GaN epilayer with $d_{\text{B}} \gg d_0$ on the In content x and the misfit dislocation density, $N^{\text{misfit}}_{\text{d}}$, calculated on the basis of Eqs. (3) and (4), is shown in Fig. 1. The calculations have been performed with parameters for GaN and InN given in Ref. [1], and use of the linear interpolation for evaluation of the parameters inside the $\text{In}_x\text{Ga}_{1-x}\text{N}$ well.

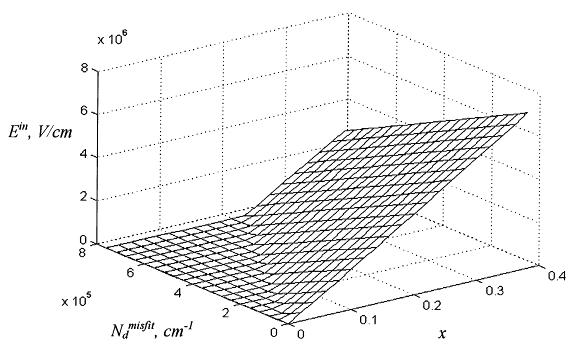

Fig. 1. The dependence of the built-in electric field inside the $\text{In}_x\text{Ga}_{1-x}\text{N}$ quantum well embedded in GaN epilayer on the In content x and the misfit dislocation density, $N^{\text{misfit}}_{\text{d}}$.

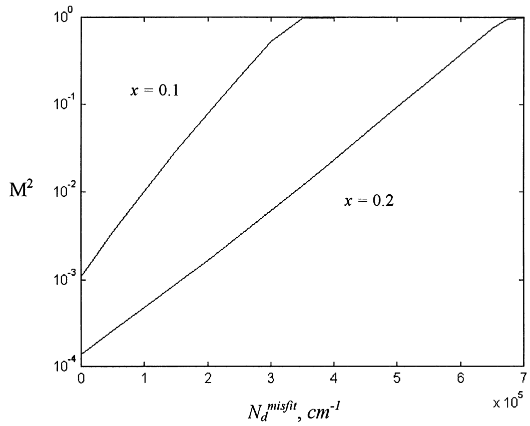

Fig. 2. The dependence of the overlap integrals M^2 on the concentration of the misfit dislocation calculated for the intrinsic $\text{In}_x\text{Ga}_{1-x}\text{N}$ quantum well structure with the well width $d_{\text{W}} = 40$ Å and In content $x = 0.1$ and 0.2.

The $\text{In}_x\text{Ga}_{1-x}\text{N}$ quantum well shapes the wave functions for electrons and holes in the wells, and the squares of the overlap integrals M^2 between the electron and the hole wave functions are calculated for the well width $d_{\text{W}} = 40$ Å and In contents $x = 0.1$ and 0.2. The corresponding dependence of the overlap integrals M^2 on the concentration of the misfit dislocation is shown in Fig. 2. It can be seen that the misfit dislocations can enhance the radiative recombination rate by more than 1000 times.

To find out which density of the misfit dislocations is optimal for radiative efficiency and performance of the light emitting devices with $\text{In}_x\text{Ga}_{1-x}\text{N}$ quantum wells, we need to account for their contribution to the nonradiative recombination. For this, we will use the approach that we have earlier developed for calculations of the diffusion-limited nonradiative recombination activity of the threading dislocations in GaN crystals [2,3]. According to Ref. [3], the internal quantum efficiency η of volume GaN crystals with threading dislocations is given by

$$\eta = \tau_{\text{r}}^{-1} / \left(\tau_{\text{r}}^{-1} + \tau_{\text{threading}}^{-1}\right) = \left\{1 + 4\pi D N^{\text{threading}}_{\text{d}} / Bn\left[\ln\left(1/\pi N^{\text{threading}}_{\text{d}} r_0^2\right) - 6/5\right]\right\}^{-1} \tag{5}$$

where τ_{r} is the radiative recombination time, $\tau_{\text{threading}}$

is the diffusion-limited nonradiative recombination time at threading dislocations, D is the carrier diffusion coefficient, $N_d^{threading}$ and r_0 are the threading dislocation density and capture radius, B is the van Roosbroek and Shockley radiative constant and n is the carrier concentration. The diffusion-limited recombination time at the misfit dislocations in quantum wells, τ_{misfit}, found from the solution of 2d-diffusion equation is

$$\tau_{misfit} = 1/4D\left(N_d^{misfit}\right)^2 \tag{6}$$

Eq. (5) can be easily generalized to account for the τ_{misfit} given in Eq. (6), and this gives the following expression for internal quantum efficiency of the quantum well

$$\eta = \frac{\tau_r^{-1}}{\tau_r^{-1} + \tau_{threading}^{-1} + \tau_{misfit}^{-1}} = \frac{1}{1 + \frac{4dD}{M^2 B n_{2d}}\left\{\frac{\pi N_d^{threading}}{\ln\left(\frac{1}{\pi N_d^{threading} r_0^2}\right) - \frac{6}{5}} + \left(N_d^{misfit}\right)^2\right\}} \tag{7}$$

where n_{2d} is the 2d-carrier concentration in the quantum well, which is related to the injection current density, j, by the equation

$$j = e n_{2d}\left\{\frac{M^2 B n_{2d}}{d} + \frac{4D\pi N_d^{threading}}{\ln\left(\frac{1}{\pi N_d^{threading} r_0^2}\right) - \frac{6}{5}} + 4D\left(N_d^{misfit}\right)^2\right\} \tag{8}$$

The dependence of the internal quantum efficiency on the concentration of misfit dislocations calculated, on the basis of Eq. (8), with parameters $D = 0.12$ cm^2/s [5], $B = 1.1 \times 10^{-8}$ cm^3/s [6], $N_d^{threading} = 5 \times 10^{10}$ cm^{-2} and $r_0 = 10^{-7}$ cm for two quantum wells with the same width $d = 40$ Å and In contents $x = 0.1$ and 0.2, is shown in Fig. 3. It can be seen from this figure that the misfit dislocations with densities $\sim 10^{5-6}$ cm^{-1} can improve the quantum efficiency many times due to the reduction of the built-in electric field. At higher densities, the misfit dislocations suppress the quantum efficiency since they produce an additional channel of nonradiative recombination. The optimal misfit dislocation density depends on the injection current density, and depth and width of the quantum well.

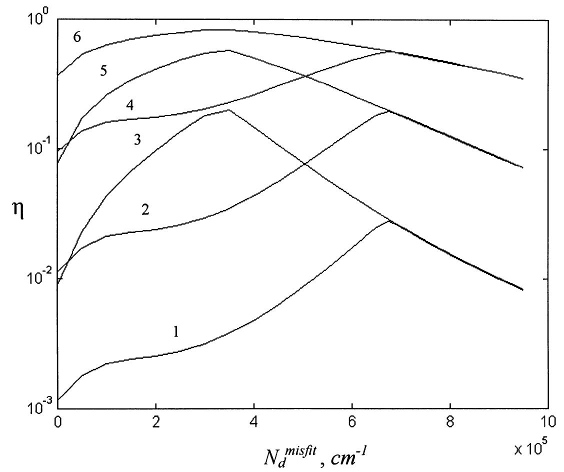

Fig. 3. The dependence of the internal quantum efficiency η on the concentration of the misfit dislocation N_d^{misfit} in the $In_xGa_{1-x}N$ well. (1) $j = 10^4$ A/cm^2, $x = 0.2$; (2) $j = 10^4$ A/cm^2, $x = 0.1$; (3) $j = 10^5$ A/cm^2, $x = 0.2$; (4) $j = 10^5$ A/cm^2, $x = 0.1$; (5) $j = 10^6$ A/cm^2, $x = 0.2$; (6) $j = 10^6$ A/cm^2, $x = 0.1$.

Thus, the radiative efficiency of the carriers in quantum wells is very sensitive to the interface quality and is not in monotone dependence with the density of the misfit dislocations in contrast to the threading dislocation case.

Acknowledgements

Y.T. Rebane and Y.G. Shreter thank the Russian Fund of Fundamental Studies for support.

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