Effect of heterointerface polarization charges and well width upon capture and dwell time for electrons and holes above GaInN/GaN quantum wells

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(Received 11 December 2009; accepted 2 March 2010; published online 29 March 2010)

The dwell time of electrons and holes above GaInN/GaN quantum wells is calculated using the $k \cdot p$ quantum transmitting boundary method. A long dwell time is an indication for high probability of carrier capture by the quantum well. Conversely, a reduced dwell time indicates that the carrier is likely to be coherently transported across the well. It is shown that sheet charges at GaInN/GaN heterointerfaces and a narrow quantum well lead to significant reductions in carrier dwell time. In addition, carrier capture is discussed in terms of a classical model that is consistent with dwell time calculations. © *2010 American Institute of Physics*. [doi:10.1063/1.3373610]

The transport characteristics of electrons and holes in GaN are known to be substantially different. High electron concentrations are achievable with the n-type dopant Si due to its relatively low ionization energy of about 20 meV,[1] and electron mobility is fairly high, with values above 200 $cm^2\ V^{-1}\ s^{-1}$ being typical for n-type GaN.[1] By contrast, high hole concentrations are generally not achievable due to the large ionization energy of the p-type dopant Mg in GaN, which has been estimated at 120 meV.[2] In addition, hole mobility is typically on the order of 10 $cm^2\ V^{-1}\ s^{-1}$ for doped p-type GaN.[3] Further, sheet charges that arise from the discontinuity in material polarization at heterointerfaces in GaN-based light-emitters grown along the c-direction also have a profound effect upon carrier transport. Previously, it has been proposed that such transport-related characteristics give rise to the rapid decrease in efficiency observed in GaN-based light-emitting diodes (LEDs) once the current density exceeds only a few amperes per square centimeter.[4] This phenomenon, known as efficiency droop, is a severe problem particularly for high-power LEDs intended for solid-state lighting. In addition to transport-based explanations of the efficiency droop, other causes have been suggested, including delocalization of carriers from In-rich low-defect-density sites[5,6] and Auger recombination[7,8] occurring at high current densities.

Motivated by these different explanations, several modified LED structures designed to reduce efficiency droop have been realized as follows: LEDs with quantum barriers (QBs) consisting of GaInN or AlGaInN were shown to reduce polarization charges at the quantum well (QW) interfaces, and to deliver improved high-current efficiency with a reduced droop in efficiency.[10,11] LEDs with only a single, very wide QW were also shown to have improved efficiency at high currents;[9] the increased QW width was intended to decrease carrier density and reduce Auger recombination. While such results are highly encouraging, they do not constitute definitive evidence that one particular mechanism is indeed the dominant mechanism causing droop; undoubtedly, either of these modifications of the LED active region structure will affect both the carrier density in the active region in addition to carrier transport.

The present letter aims to add to the understanding of carrier transport in GaN-based visible light-emitters and its effect upon efficiency. Specifically, we focus on carrier capture by QWs in the presence of polarization fields. We first consider a classical analysis of carrier capture by a QW, and then proceed to treat the quantum-mechanical carrier dwell time above a QW and its dependence on polarization and QW width.

From a classical point of view, electron capture occurs in nonpolar QWs even for very small energy losses incurred by the carrier while propagating above a QW. However, in polar structures, as shown in Fig. 1, a minimum energy loss is required due to the unequal height of the left-hand-side and right-hand-side QBs. A basic analysis can be performed by assuming that electrons launched from the barrier into the QW travel at the saturation velocity ($v_{sat} \approx 10^7$ cm s^{-1}), and lose energy through longitudinal optical (LO) phonon emission ($E_{LO} \approx 92$ meV, $\tau_{LO} \approx 0.01$–0.2 ps), which yields an energy loss of 14–280 meV for a 3 nm wide QW. Simulation results indicate that the conduction band edges of the left and right QBs of blue-emitting $Ga_{0.8}In_{0.2}N$ QWs may be separated by several hundred millielectron volt; therefore, incomplete capture of carriers by QWs is possible. We note that as the In composition in the QW is increased, the electric field in the QW increases, and the minimum energy loss for capture will also increase. Therefore, capture is less likely for QWs emitting at longer wavelengths.

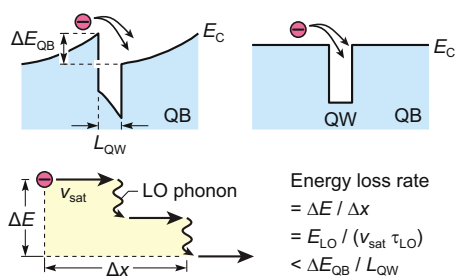

FIG. 1. (Color online) Illustration of electron capture process in QWs.

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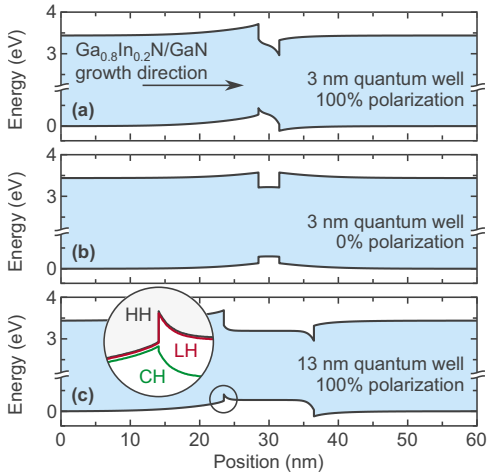

FIG. 2. (Color online) Calculated band diagrams of $Ga_{0.8}In_{0.2}N/GaN$ QWs grown in the c-direction. (a) 3 nm GaInN well with full theoretical polarization; (b) 3 nm GaInN well with zero polarization; (c) 13 nm GaInN well with full theoretical polarization.

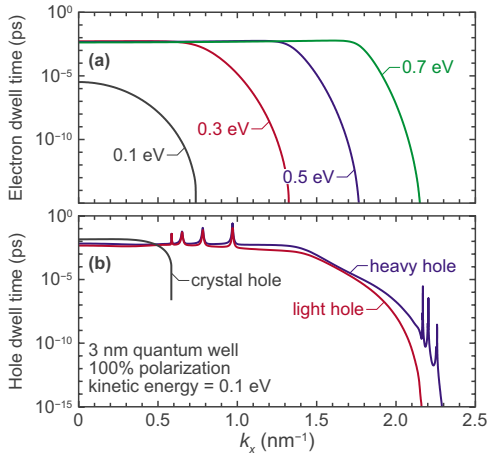

FIG. 3. (Color online) (a) Calculated dwell times as a function of the in-plane wave vector for electrons with different kinetic energies above a 3 nm QW with full theoretical polarization. (b) Calculated dwell times for incident heavy hole, light hole, and crystal hole states with 0.1 eV kinetic energy.

Next, we extend the classical analysis by presenting a theoretical study of the dwell time, τ_d, of electrons and holes above a QW. A dwell time is associated with each allowed wave function, and reflects the time that a carrier in a particular wave function resides above the QW, assuming coherent transport and no phonon emission. Dwell time is distinct from the capture time of carriers; given the capture time τ_c and the electron density n, the total transition rate of electrons into a QW can directly be found by n/τ_c. The dwell time gives more general information about the shape of a wave function in the vicinity of a QW. In a diode under forward bias, the net current is due to diffusion of carriers. As a carrier is transported by diffusion, it is repeatedly scattered and transitions among states. The direction of travel may be randomized with every scattering event, and therefore the actual time that a carrier spends within a region can be large. However, this time will still be related to the dwell times of the wave functions among which the carrier transitions. The dwell time is given by,

$$\tau_d = \frac{1}{J_{inc}} \int_{qw} |\psi|^2 dz, \tag{1}$$

where ψ is an incident wave function, J_{inc} is the incident probability current density, the integral is over the width of the QW, and the z-direction is the growth direction.[12] A longer dwell time can be expected to yield higher probability of scattering from an unbound incident state into a bound state in the QW, i.e., capture of carriers by the QW. Possible mechanisms for this capture of electrons include optical phonon emission as well as impurity and acoustic phonon scattering.[13]

The structure used in our calculations consists of a $Ga_{0.8}In_{0.2}N$ QW surrounded by n-type GaN with a dopant concentration of 1×10^{18} cm^{-3}. Growth in the c-direction is assumed. The band diagram under nonequilibrium conditions is calculated by self-consistent solution of Poisson's equation including material polarization and the continuity equations for electrons and holes.[14,15] Figure 2 shows the band diagrams for three example structures. Although the calculation of the band diagram and carrier distribution is purely classical, it is expected that the electrostatic potential found by this method reasonably approximates the actual potential in the vicinity of GaInN/GaN QWs. Once the potential has been found, wave functions are calculated using the $k\cdot p$ quantum transmitting boundary method[16] with an 8×8 Burt–Foreman Hamiltonian. The quantum transmitting boundary method has also been applied to find transmission coefficients through interband polarization-charge tunnel junctions;[14,17] a detailed discussion of this method is given in Ref. 14.

Figure 3(a) shows the electron dwell time above the QW for the structure in Fig. 2(a) at several different kinetic energies as a function of the in-plane wave vector. Dwell times are independent of the wave vector direction due to the axial symmetry in the dispersion relation for the conduction band. At larger kinetic energies, the dwell time is approximately constant over a range of wave vector magnitudes, and then gradually decreases as the in-plane wave vector increases. This can be understood in terms of the kinetic energy along the growth direction; wave functions with greater kinetic energy in the growth direction are hindered less by the barrier to injection seen in Fig. 2(a), which results in greater wave function amplitude in the well and a longer dwell time. Figure 3(b) shows the dwell time for holes in the HH, LH, and CH band above the QW for the structure in Fig. 2(a). The kinetic energy in all cases is 0.1 eV. For each band, the general behavior of dwell time as a function of in-plane wave vector roughly matches that of electrons. However, at the same kinetic energy, dwell times for holes are significantly longer. Further, the dwell times for the HH and LH bands feature sharp peaks, which are connected with strong mixing of the bands.[12] A series of peaks occurs in both the HH band and LH band when the kinetic energy of the CH band is entirely in the in-plane direction; an additional series is found in the HH band when the kinetic energy of the LH band is entirely in the in-plane direction.

Assuming that the occupation of incident electron and hole states is described by separate, single quasi-Fermi levels, all states with a particular energy will have equal occupation probability. For a particular energy, then, an average dwell time can be calculated by integrating the dwell time over the allowed in-plane wave vector values. Figure 4(a) plots the average dwell times for electrons over a QW for the structure in Fig. 2(a), as well as the same structure with material polarization reduced to 50% of its theoretical value,

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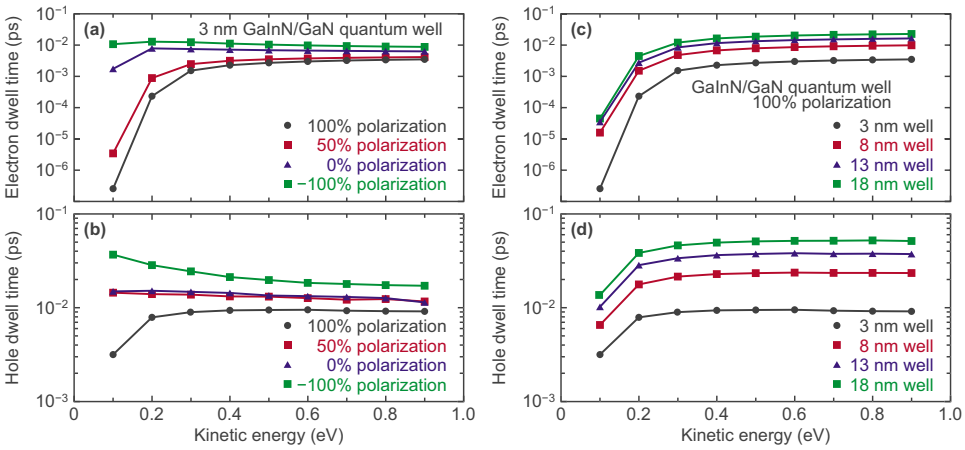

FIG. 4. (Color online) (a) Calculated average electron dwell times as a function of kinetic energy for $Ga_{0.8}In_{0.2}N/GaN$ QWs with 3 nm width and various polarization values. (b) Calculated average hole dwell times for the same cases. (c) Calculated average electron dwell times as a function of kinetic energy a $Ga_{0.8}In_{0.2}N/GaN$ QWs with full theoretical polarization and various well widths. (d) Calculated average hole dwell times for the same cases.

zero polarization [as shown in Fig. 2(b)], and with inverted polarization. Elimination of the polarization results in increased dwell time for all values of kinetic energy, but particularly at low energies. When the kinetic energy of the incident electron is 0.1 eV, dwell time is increased by four orders of magnitude, compared to less than one order of magnitude at energies above approximately 0.5 eV. Partial elimination of the polarization mismatch still has a significant effect; at low energies, the dwell time for electrons in partially polarization-matched structures increases by approxiamtely a factor of 10.

Complete inversion of polarization results in the longest dwell times at all energies. The structure with inverted polarization is identical to that of Fig. 2(a) when flipped about the vertical axis. In this case, rather than increasing the barrier to injection, the sheet charges at heterointerfaces act to lower the barrier for injection and create a barrier for transmission through the well. The increase in dwell time is particularly pronounced for electrons with low kinetic energy, as these are affected most by the change in the potential. Figure 4(b) plots the average dwell times for holes over a QW for the same cases shown in Fig. 4(a). Overall, when compared to the electron dwell time, the hole dwell time is larger, and does not depend as strongly upon the carrier kinetic energy. As for electrons, eliminating or inverting polarization results in increased dwell time for holes at all energies. However, unlike for electrons, the structure with 50% of theoretical polarization has nearly the same dwell times at all kinetic energies. This finding motivates the pursuit of growth of polarization-inverted structures which can be attained for N-face growth or p-side down structures on c-plane sapphire.

Next, the effect of quantum-well width upon dwell time is considered. Figure 4(c) plots the electron dwell times over a QW as a function of kinetic energy for well widths ranging from 3 to 18 nm. Figure 4(d) plots the hole dwell times for the same cases. Inspection of the figure shows that the dwell time is increased for both electrons and holes as the QW width increases. Due to the injection barriers induced by the polarization charges, dwell times for low kinetic energies remain short compared to the zero-polarization and inverted-polarization cases in Figs. 4(a) and 4(b). Nevertheless, increasing well width results in strongly increased dwell times, by up to two orders of magnitude. This suggests that a major benefit of wider wells is found in more efficient capture of carriers by the QW.

In summary, carrier capture in GaInN QWs is analyzed using a classical model, which indicates a reduced carrier capture probability for polar QWs. In addition, the quantum-mechanical dwell time of electrons and holes above QWs is investigated using the quantum transmitting boundary method and the 8×8 Burt–Foreman Hamiltonian for wurtzite III-nitride semiconductors. The results indicate that both reduction in heterointerface polarization charges and increasing of QW width increase electron and hole dwell time over QWs, and thereby increase the probability of capture of carriers by the QWs.

This material is based upon work supported by the National Science Foundation under Grant No. DMR-0642573, by NYSTAR under Contract No. C070119, and by Sandia's Solid-State Lighting Science Center, an Energy Frontier Research Center funded by the U. S. Department of Energy, Office of Science and Office of Basic Energy Sciences.

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