P:17 Monte Carlo analysis of impact ionization processes and band-to-band tunneling in InxGa1-xAs PIN ungated devices

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Impact-ionization (II) metal-oxide-semiconductor FETs (I-MOSFETs) [1] are in competition with tunnel-FETs (TFETs) [2] to achieve the best behavior for ultra-low subthreshold-swing (SS) logical circuits. In particular, narrow-bandgap III-V I-MOSFETs are being explored as promising devices because of the low values of SS and ON-state drain-to-source voltage V_{DS}. However, in III-V structures band-to-band tunneling emerges for lower applied V_{DS} than II processes, thus hindering the development of III-V I-MOSFETs.

In order to facilitate the design process of III-V I-MOSFETs from the physical point of view, this work reports the development of a Monte Carlo (MC) simulator able to reproduce the internal quantities of ungated diodes at the basis of I-MOSFETs or TFETs. Our simulator incorporates the II events by means of the Keldysh approach [3], where the probability per unit time of having an II process is $P\ (E) = S\ [(E\ -\ E_{th})/\ E_{th}]2$ when $E > E_{th}$, E being the electron kinetic energy, E_{th} the ionization threshold energy and S a measure of the softness or hardness of the threshold. To take into account band-to-band tunneling, the transmission coefficient T_C along the longitudinal dimension is determined for each energy following the Wentzel-Kramers-Brillouin (WKB) method, considering the shape of the energy barrier provided by MC simulations [4]. The expression for the transmission coefficient involves a global proportionality constant K that includes, among other quantities, the electron and hole effective masses during the tunnel transmission and the Richardson constant [4]. Both S and K are typically considered as adjustable parameters to reproduce the experimental I-V curves. This MC model has been validated by comparison with the experimental measurements of an ungated $In_{0.53}Ga_{0.47}As$ 100 nm PIN diode, using S=2x10^{12} s^{-1} for $P(E)$ and K=10^{21} Am^{-1}s^{-1} for T_C.

The internal quantities of $In_{0.53}Ga_{0.47}As$, $In_{0.7}Ga_{0.3}As$ and InAs ungated PIN devices have been evaluated considering tunnel events or II processes independently, at the onset of the ON-state current. To illustrate these results, Fig. 1 presents the MC values of the number of electron-hole pairs generated by tunnel events or II processes and the energy bands for -3.1 V applied to the $In_{0.7}Ga_{0.3}As$ structure. Tunneling, linked to the shape of the energy bands, is responsible for the onset of I_{ON}, the threshold voltage V_{T_tunnel} being about -2.8 V, much lower than that found for In0.53Ga0.42As, around -3.8 V. When considered in the simulations, II processes, originated by electrons coming from the p-side of the device, take place mainly in the n-side of the intrinsic area and the n+ region. The value of V_T linked to II events is $V_{T\_II} \sim -3.1$ V, while in the In0.53Ga0.42As structure no current due to II processes is found at least up to -5.0 V when only II is considered. In case II and tunnel processes are jointly accounted for in the simulations, II processes do take place for x=0.53, triggered by tunneled carriers. Interestingly, when increasing the proportion of In, thus reducing the bandgap, the decrease in V_{T_II} is much more pronounced than that in V_{T_tunnel}. Semiconductors with lower bandgap, as InAs and InSb, must be analyzed to check if II can dominate the onset of the current.

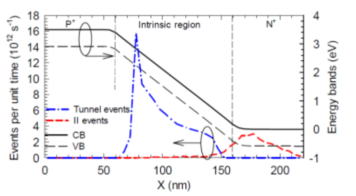

Fig. 1. MC values of the electron-hole pairs generated by tunnel events or II processes curves per unit time and energy bands for -3.1 V for the $In_{0.7}Ga_{0.3}As$ 100 nm PIN diode, being S=2x10^{12} s^{-1} and K=10^{21} Am^{-1}s^{-1}.

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P:18 Multi-scale nonequilibrium green's function method for LEDs: Balance of thermalization and tunneling

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GaN/InGaN multi-quantum-well (MQW) structures are the core technology of most mid-to-high power blue light-emitting diodes (LED). Their optimization requires a quantitative understanding of the nanoscale carrier flow. Typical LEDs are characterized by high carrier density regions such as n-GaN/p-GaN leads and InGaN quantum wells (QW). The charge transport is based on both tunneling and thermionic emission. In this work, a multi-scale quantum transport model for efficient and quantitative modeling of a commercial LED is applied [1,2] and augmented to include nonlocal quantum effects. This method is based on the nonequilibrium Green's function (NEGF) formalism to compute the dynamics (states) and the kinetics (filling of states) in the entire extended complex device. The model results agree with experimental I-V curves quantitatively. In this work, we provide a quantitative assessment of long-range tunneling in LEDs. II.

The methodology is based on carrier scattering versus carrier tunneling oriented partitioning of the device as shown in Fig. 1. The n-GaN/p-GaN layers and QWs have extremely high carrier densities. Since the carrier scattering is very strong in these regions, they are considered local equilibrium carrier reservoirs with local quasi Fermi levels. In each reservoir, an imaginary optical potential (η = 0.1eV according to photoluminescent (PL) measurements [3]) is included in the diagonal of the Hamiltonian [4] to mimic the scattering. Current conservation is ensured by self-consistently solving the local Fermi levels [2]. Figure 1 shows all current paths through barrier #4 as an example. In the previous work, all the current paths coupling more than two QW were not considered. In this work, the model is expanded to allow for transport current coupling multiple QWs. 'Hot carrier' formation is allowed in this way. III.

The model is applied to simulate a commercial GaN/InGaN blue LED (see Fig. 1). Figure 2 plots the electron and hole densities with band diagrams and local Fermi levels. Electrons are well transported across the MQW, as indicated by low Fermi level drop (~25meV) and well spread-out carrier distribution. In contrast, the hole Fermi level drop (~180meV) is much larger and as a result the hole distribution is skewed towards the p-side. A realistic (0.1eV) and a reduced (0.01eV) η value were simulated and compared. For each η, two sets of simulations were performed. The first set (denoted as 'short') includes only nearest neighbor QW currents. The second set (denoted as 'long') includes all transport components across different QWs. Larger η leads to higher thermionic emission due to more broadened states. The majority of current conduction occurs below the barriers, and decays significantly with longer coupling range. Figure 3 and 4 compares the I-V and internal quantum efficiency (IQE) for different η values and coupling ranges. For larger η, the IQE droops became worse. This is because higher scattering reduces the mobility in the QWs, which leads to more holes piling up at the p-side (see Fig. 2) and thus increases nonradiative losses. The I-V at 0.1eV agrees quantitatively with experimental results. The effect of long-range coupling is only observable at low scattering case (η=0.01eV). Realistic thermalization in LEDs prevent the hotcarrier formation.

An efficient, multi-scale NEGF based transport model was applied on a commercial LED structure. Complete thermalization in the LED QWs has been confirmed. Reducing the scattering rate by 1 order of magnitude, however, allows for the formation of 'hot carriers' due to long range tunneling.