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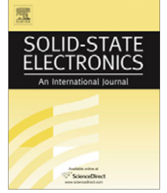

Multiple steady state current–voltage characteristics in drift–diffusion modelisation of N type and semi-insulating GaAs Gunn structures

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ABSTRACT

Theoretical and numerical investigations of carriers transport in N–Semi-Insulating (SI)–N and P–SI–P diodes is extended to the case of extrinsic (N type) or SI samples with Gunn like electric field dependent mobilities. The results obtained in a preceding publication [1] are valid as long as the bulk electric field does not increase above a threshold field E_{th} associated with the beginning of negative electron differential mobility values: $\mu_{n,diff} = (dv_n/dE) < 0$, v_n being the electron drift velocity. Convergence and stability problems occur only, for the steady state numerical simulation, in long N^+–N–N^+ or N^+–SI(N^-)–N^+ diodes. SI(N^-) characterizes a SI layer which keeps, under applied bias, a free electron concentration close to its thermal equilibrium value up to the beginning of electron space charge injection. A systematic study has been made by varying the contact boundary properties: flat band, metallic, N^+ or P^+; the length of the sample and the electric parameters of the deep compensating trap of the SI layers. We show that these steady state numerical instabilities are related to the existence of multiple current–voltage solutions when numerical modelisation is made using the drift–diffusion model.

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1. Introduction

In a previous article [1], we analyzed ambipolar conduction mechanisms in N–Semi-Insulating (SI)–N and P–SI–P structures. We used the analytical and numerical framework of the drift–diffusion model with constant electron and hole mobilities. Both long samples, $L_{SI} > L_{Da}$ as used for radiation detectors and short samples, $L_{SI} < L_{Da}$ as used in buried heterostructures, were considered, L_{SI} being the SI layer thickness and L_{Da} the ambipolar diffusion length.

SI GaAs or InP are obtained by deep level compensation of residual donors or acceptors. The deep centre and residual donor or acceptor concentration values: N_t, $|N_A - N_D|$, are in the range 10^{15}–10^{17} cm^{-3} and for carrier lifetimes of the order or greater than 10^{-9} s, L_{Da} is greater than both the contact (N–SI or P–SI) space charge thicknesses and the screening length L_S [2]. For a mid-gap deep level and a compensation ratio $r = |N_A - N_D|/N_t \approx 0.5$, L_S reduces to:

$$L_S = \sqrt{\frac{\varepsilon_0\varepsilon_r kT}{e^2(n_e+p_e)}}\left[1+\frac{N_t n_e p_e}{(n_e+n_{1t})(p_e+p_{1t})(n_e+p_e)}\right]^{-\frac{1}{2}} \approx \sqrt{\frac{4\varepsilon_0\varepsilon_r kT}{e^2 N_t}} \quad (1)$$

Typical L_S values, for $N_t \in [10^{15}$–10^{17} cm$^{-3}]$ and $T = 300$ K, are in the range [100–10 nm]. For short SI layers, having thicknesses L_{SI} of the order or less than one μm, it is difficult to distinguish contact from bulk effects.

Equilibrium free carrier densities: n_e, p_e in SI layers are obtained assuming space charge neutrality and complete ionization of shallow donors or acceptors. In the case of a deep donor, density N_t, compensating a residual acceptor of density N_A with p_{te} the equilibrium concentration of ionized deep donor centres, the space charge density $\rho_{sc} = e(p_e + p_{te} - n_e - N_A) = 0$. With n_e, $p_e \ll N_A < N_t$, we have $p_{te} \approx N_A$, leading to:

$$n_e \approx n_{1t}\left[\frac{N_t}{N_A}-1\right] \quad \text{and} \quad p_e \approx p_{1t}\left[\frac{N_t}{N_A}-1\right]^{-1} \quad (2)$$

Equivalent relations are found for the case of a deep acceptor level compensating a residual donor.

An important relation, valid outside the space charge regions, was obtained for non-equilibrium conditions between the excess free carrier densities $\Delta n = (n - n_e)$ and $\Delta p = (p - p_e)$ [1]:

$$\alpha_t = \frac{\Delta n}{\Delta p} \approx \frac{\tau_{nt}}{\tau_{pt}}\left[\frac{N_t - N_A}{N_A}\right] = \frac{\tau_{nt}}{\tau_{pt}}\frac{n_e}{n_{1t}} \quad (3)$$

where τ_{nt}, τ_{pt}, p_{1t} and n_{1t} are the Shockley–Read–Hall trap parameters with: $n_{1t}p_{1t} = n_e p_e = n_i^2$ [3]. Eq. (3) is valid in the case of field dependent mobilities. It is an extension, for SI layers, of the well known quasi space charge neutrality condition, $\Delta n \approx \Delta p$,

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valid in the steady state and outside space charge regions, for extrinsic semiconductors. This relation is verified for lifetime semiconductors [4], where $L_S \ll L_{Da}$. This is the case of compensated SI GaAs and InP. Before the onset of one carrier space charge current at high injection level the free carrier concentrations n and p are negligible for N–SI–N and P–SI–P structures and the space charge reduces to $\rho_{sc} \approx e(p_t - N_A)$. Eq. (3) can be deduced from the steady state value of the ionized deep donor concentration $p_t(n,p)$:

$$p_t(n,p) = N_t[\tau_{nt} p + \tau_{pt} n_{1t}]/[\tau_{nt}(p + p_{1t}) + \tau_{pt}(n + n_{1t})] \quad (4)$$

Differentiating, $dp_t = 0$ gives Eq. (3). It was shown [1] that for any increment Δn and Δp verifying Eq. (3) we have: $\Delta p_t = (p_t - p_{te}) = 0$ and $\rho_{sc} \approx 0$. This space charge neutrality condition breaks down inside the contact space charge region and at the beginning of electron or hole space charge currents.

Starting with Eq. (3) together with the familiar Shockley hypothesis of quasi Boltzmann equilibrium across N–SI contacts: $n_{SI} \approx n_{SI,e} \exp(eV_j/kT)$ or P–SI contacts: $p_{SI} \approx p_{SI,e} \exp(eV_j/kT)$, another useful relation was established involving a parameter M_t, a simple function of the deep centre electrical parameters:

$$M_t = \frac{N_A}{(N_t - N_A)} \frac{\tau_{nt}}{\tau_{pt}} \frac{p_{1t}}{n_{1t}} \quad (5)$$

When $M_t < 1$, the SI layer behaves like a SI(N^-) layer and a linear J–Va relationship is observed for N–SI(N^-)–N structures at low and intermediate applied voltage. The conduction mechanism is bulk controlled with the electric field $E \approx |Va|/L_{SI}$, the conductivity $\sigma \approx \sigma_{ne}$ together with negligible voltage drops, V_{j1} and V_{j2}, across both N–SI contacts. Both contacts show ohmic behaviour. For increasing applied bias $|Va|$, complete depletion of holes ($\Delta p \approx -p_e$) may occur together with a barely affected electron concentration, if $M_t \ll 1$ [1]. At higher voltage, electron space charge current set in. For a P–SI(N^-)–P structure, on the other hand, the J–Va relationship shows a saturation effect. Most of the applied voltage is lost across the reversed biased contact and hole space charge current sets in at higher voltage. It is important to note that a SI(N^-) layer can be such as to satisfy $p_e > n_e$, i.e. a SI(N^-) layer can be in fact P type at thermal equilibrium with $\sigma_e \approx \sigma_{pe}$.

When $M_t > 1$, the SI layer behaves like a SI(P^-) layer. P–SI(P^-)–P structures are bulk controlled showing a linear, quasi ohmic, $\sigma \approx \sigma_{pe}$, J–Va relationship and electron depletion occurs for increasing Va. N–SI(P^-)–N structures are contact controlled. The SI(P^-) layer can be N type at thermal equilibrium with $n_e > p_e$ and $\sigma_e \approx \sigma_{ne}$.

When $M_t \approx 1$, typically for $0.5 \leqslant M_t \leqslant 2$, both contacts and bulk effects are important. The transition from ohmic regime (bulk controlled) to saturation regime (contact controlled) is quite swift around $M_t = 1$, see Fig. 8 [1].

2. Drift–diffusion equations with electric field dependent mobilities

2.1. Electric field dependent mobilities

We now extend our analysis to the case of electric field dependent mobilities and drift velocities [5–9], with:

$$v_n = \mu_n(E)E = \frac{\mu_{no}E + v_{n,sat}\left[\frac{E}{E_o}\right]^4}{1 + \left[\frac{E}{E_o}\right]^4} \quad (6)$$

$$v_p = \mu_p(E)E = \frac{\mu_{po}E}{1 + \left[\frac{\mu_{po}E}{v_{p,sat}}\right]} \quad (6\text{bis})$$

$\mu_{no} = 4000\ \text{cm}^2/\text{Vs}$ and $\mu_{po} = 280\ \text{cm}^2/\text{Vs}$ are the low electric field mobilities, $v_{n,sat} = 8.5 \times 10^6$ cm/s, $v_{p,sat} = 10^7$ cm/s the saturation drift velocities and $E_o = 4000$ V/cm. In this model, v_p is a continuously increasing function of E up to its saturation value $v_{p,sat}$. The electron velocity, on the other hand, show a broad maximum value, $v_{n,max} \approx 1.22 \times 10^7$ cm/s, obtained at a threshold electric field value $E_{th} \approx 4080$ V/cm. This is followed by a region of pronounced negative differential mobility, $\mu_{n,diff} = (dv_n/dE) < 0$, in the interval $E \in [4–10\ \text{kV/cm}]$. Above $E \approx 10$ kV/cm, $v_n \approx v_{n,sat}$. From Eq. (6) we obtain the following relation: $v_{n,max} = (3\mu_{no}E_{th})/4$.

In an electrically homogeneous semiconductor, such as N GaAs or InP layers, when $\mu_{n,diff} < 0$ and if contact effects can be neglected, a local charge fluctuation is amplified resulting in the formation of a high field domain and high frequency Gunn oscillations [10–12]. For a trap controlled SI layer, instabilities and low frequency oscillations are observed [13 and ref. therein]. These instabilities can be cyclic or even chaotic and occur on various time-scales. In particular for a SI compensated sample, using time dependent analysis, we have for the ionized deep donor concentration $p_t(n, p)$:

$$\frac{\partial p_t}{\partial t} + \frac{p_t}{N_t} \frac{\tau_{nt}(p + p_{1t}) + \tau_{pt}(n + n_{1t})}{\tau_{nt}\tau_{pt}} = \frac{\tau_{nt} p + \tau_{pt} n_{1t}}{\tau_{nt}\tau_{pt}}.$$

For the steady state it reduces to Eq. (4). Now, assuming small departure from the steady state: n_o, p_o, the reduced (homogeneous) equation has a solution: $p_t \sim \exp(-t/\tau_r)$ with the characteristic time $\tau_r = \tau_{nt}\tau_{pt}N_t/[\tau_{nt}(p_o + p_{1t}) + \tau_{pt}(n_o + n_{1t})]$. τ_r is of the order of $\tau_{nt}(N_t/n_e)$ with a value equal to a few seconds in the case of SI GaAs or InP having a mid-gap deep level and similar hole and electron capture cross sections. If we assume that the electric field is homogeneous (spatially uniform) and has the same value in the bulk and near the contact, we do not expect, for time independent conditions, a Gunn N type negative resistance to lead to numerical instabilities in computer simulation under constant bias Va.

Eq. (6) assumes quasi instantaneous intervalley relaxation time. This leads to other difficulties. At first, for very short, ballistic devices, the effect of the electric field is known to be non local and this $v_n(E)$ relationship should then be applied to transport problem with care [11, p. 62 and 10, p. 652]. This is not a problem for our somehow longer samples. Then, numerical instabilities and lack of convergence towards a stable numerical solution is often reported for inhomogeneous samples in the steady state and under constant dc bias when $\mu_{n,diff} < 0$; leading some authors to resort to a simple velocity saturation model [14,15]. We will try below to clarify the difficulties related to numerical instabilities.

It is well known that, due to contact effect, there is a large discrepancy between the average, sometimes called the configurational electric field, defined as the ratio of the applied voltage to the sample length and the real, position dependent, field value [10, p. 651, 16,17]. In order to assess the origin of the numerical instabilities observed in our samples, we will first consider samples such that at thermal equilibrium we have a flat band structure. We will consider both N and compensated SI layers and we will show that, for these thermal equilibrium flat band structures, besides the trivial $J(Va)$ relationship associated to an homogeneous electric field $E = |Va|/L$, other physical solutions exist corresponding to position dependent E, n and p values. We believe it explains the numerical instabilities observed for the more complex samples such as N^+–N–N^+ and N^+–SI–N^+ structures.

2.2. Physical and numerical model: time independent drift–diffusion equations

We take into account, in the framework of the drift–diffusion model, the Shockley–Read–Hall generation recombination mechanism as well as the trapped space charge:

$$\rho_{sc}(x) = e[p(x) - n(x) + N_D - N_A + p_t(x) - n_r(x)] \quad (7)$$

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