



Theoretical and numerical investigations of carriers transport in N-semi-insulating-N and P-semi-insulating-P diodes – A new approach

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ABSTRACT

A new and simple theoretical model is developed for ambipolar transport in compensated N-semi-insulating (SI)-N or P-SI-P diodes and is validated with exact J – V_a characteristics obtained through numerical modelisation. The electrical parameters used correspond to SI GaAs layers, but these results are valid for other compounds such as SI InP and InGaP. A relation between the bulk non-equilibrium excess carrier concentrations, valid for low and intermediate applied voltage, is first established. For a deep donor (N_t) compensating a residual shallow acceptor (N_A): $(n - n_e) \approx \frac{\tau_{nt}}{\tau_{pt}} \left(\frac{N_t - N_A}{N_A} \right) (p - p_e)$, where n_e and p_e are the thermal equilibrium free carrier densities in the SI layer, τ_{nt} , τ_{pt} and n_{1t} , p_{1t} are the familiar Shockley–Read–Hall (SRH) parameters of the deep trap. This relation represents an extension of the well known quasi space charge neutrality condition: $(n - n_e) \approx (p - p_e)$ valid for extrinsic semiconductors. We show then that a linear J – V_a relationship is observed in N-SI-N diodes when $\mathbf{M}_t (= \frac{N_A}{N_t - N_A} \frac{\tau_{nt} p_{1t}}{\tau_{pt} n_{1t}}) < 1$ and in P-SI-P diodes when: $\mathbf{M}_t > 1$. The quasi totality of the applied voltage V_a is lost across the SI layer and the electric field is constant ($E \approx V_a/L_{SI}$). $\mathbf{M}_t < 1$ characterizes a SI(N^-) layer where a strong hole depletion ($p \approx 0$) across the SI bulk is associated to an “ohmic” electron current where n is constant but such that $n < n_e$. $\mathbf{M}_t > 1$ characterizes a SI(P^-) layer where $n \approx 0$, $p < p_e$. On the other hand, the J – V_a characteristics of N-SI(P^-)-N diodes and P-SI(N^-)-P diodes show a saturation effect. Most of the applied voltage is now lost across the reverse biased contact and the electric field is low across the SI layer. For \mathbf{M}_t values close to 1, we switch from a linear to a saturation regime. Equivalent relations are given for a deep acceptor compensating a shallow donor. We present results for short SI layers having lengths L_{SI} in the micrometer range and of the order or inferior to the ambipolar diffusion length L_{Da} , such layer are used as insulating layers in buried heterostructures for diode laser technology, as well as for long SI layers, $L_{SI} \gg L_{Da}$, as used in radiation detectors technology.

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1. Introduction

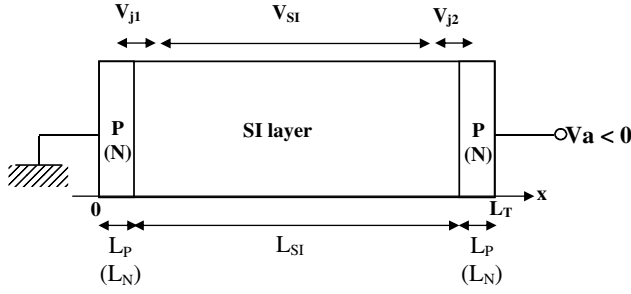
High resistivity semiconductors used in microelectronics are obtained through a mechanism called compensation in which unwanted residual donors or acceptors are neutralized (compensated) by a larger density of deep centers of the opposite type, acceptor or donor. For quasi-intrinsic behaviour the energy level of an efficient compensating center must be close to mid-gap, then the thermal equilibrium carrier densities n_e and p_e are close to their intrinsic value n_i . In this paper we will consider a deep donor level, energy E_t , density N_t , compensating a residual shallow acceptor $N_t > N_A > N_D$. Similar results are obtained for a deep acceptor level E_r , N_r compensating a residual shallow donor with $N_r > N_D > N_A$. We will show below that in the steady state, a linear relation exists across the SI layer between the excess free carrier concentrations: $\Delta n \approx \alpha \Delta p$. This relation is an extension to the quasi space charge

neutrality condition valid for extrinsic semiconductors (SC) with short dielectric relaxation time: $\Delta n \approx \Delta p$. Then, depending on the value of $\mathbf{M}_t(\mathbf{M}_r)$, a simple function of the deep level electrical parameters, the electrical behaviour of P-SI-P or N-SI-N diodes will be shown to be either bulk or contact controlled. Semi-insulating (SI) GaAs, whose room temperature electrical parameters are given in Fig. 1, is widely used as a substrate in optoelectronic devices. These substrates are obtained using Liquid Encapsulated Czochralski (LEC) or Vertical Bridgman [1,2]. For these samples, high residual density of shallow acceptors (carbon): $N_A \approx 10^{15}$ – 10^{16} cm⁻³ are compensated by a deep donor level such as the EL2 center, with concentrations is in the range 10^{15} – 10^{17} cm⁻³ with $N_t > N_A$.

Some characteristic lengths are important. The barrier space charge thicknesses w at the N-SI or P-SI boundaries are evaluated taking into account the residual donor, acceptor and deep center and neglecting the free carrier space charge. For a N-SI or P-SI contact, with a deep donor compensating a residual acceptor, the space charge thickness w across the SI layer is given for heavily doped N or P contacts by

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Total length: $L_T = L_{SI} + 2L_N(L_P)$; Applied voltage: $V_a = V_{j1} + V_{SI} + V_{j2}$

Fixed electrical parameters (GaAs):

Electron mobility: $\mu_n = 4000 \text{ cm}^2/\text{V}\cdot\text{s}$; hole mobility: $\mu_p = 280 \text{ cm}^2/\text{V}\cdot\text{s}$
 Intrinsic carrier density: $n_i = 2 \times 10^6 \text{ cm}^{-3}$; permittivity: $\epsilon_r = 12.5$; $T = 300 \text{ K}$

Variable parameters:

L_{SI} ; N_i (N_r); N_A (N_D); Energy level E_t (E_r); lifetimes: τ_{nt} , τ_{pt} (τ_{nr} , τ_{pr}).

Fig. 1. P-SI-P and N-SI-N one-dimensional structures simulated in this study.

$$w_{N-SI} \approx \sqrt{\frac{2\epsilon_0\epsilon_r(V_{Dif} - V_j)}{eN_A}} \quad \text{and} \quad w_{P-SI} \approx \sqrt{\frac{2\epsilon_0\epsilon_r(V_{Dif} - V_j)}{e(N_t - N_A)}} \quad (1)$$

where V_{Dif} is the built-in diffusion voltage and V_j the applied junction voltage. This space charge is screened out within a characteristic length L_S , usually much shorter than the intrinsic Debye length L_D . L_S arises from a spatial variation of the occupation of the deep level [3]. When the deep trap density N_t (N_r) is greater than the residual acceptor (donor) densities, L_S is very short. For a SI compensated semiconductor having a mid-gap deep level with $N_t \approx 2N_A$, such that the Fermi level is pinned to the deep energy level E_t then: $n_e \approx p_e \approx n_{1t} \approx p_{1t} \approx n_i$ and L_S reduces to

$$L_S \approx \sqrt{\frac{4\epsilon_0\epsilon_r kT}{e^2 N_t}} \quad (2)$$

At room temperature, for $N_t = 10^{16} - 10^{17} \text{ cm}^{-3}$, $L_S \leq 0.1 \mu\text{m}$. On the other hand, L_S can have large values when the compensation ratio: $r = N_A/N_t$ (or N_D/N_r) is close to 1. Taking as an example the limiting case of a mid-gap deep donor with $N_t \approx N_A$, we have $p_e \approx (p_{1t} N_t)^{1/2} \gg n_e$, n_{1t} and p_{1t} , and $L_S \approx L_D/2^{1/2}$. For $N_t = N_A = 10^{16} \text{ cm}^{-3}$ we have $L_S = 0.21 \text{ cm}$ and to the exception of very thick samples, the space charge region extends throughout the whole SI layer.

There is another important characteristic length, the ambipolar diffusion length L_{Da} [4,5]:

$$L_{Da} = \left[\frac{kT}{e} \frac{\mu_n \mu_p [\tau_{nt}(p_e + p_{1t}) + \tau_{pt}(n_e + n_{1t})]}{\mu_n n_e + \mu_p p_e} \right]^{1/2} \quad (3)$$

L_{Da} reduces to $L_{Dn} = (D_n \tau_{nt})^{1/2}$ or $L_{Dp} = (D_p \tau_{pt})^{1/2}$ for a mid-gap deep level, when p_e/n_e and $\tau_{nt} p_e / \tau_{pt} n_e \gg$ or $\ll 1$. For a SI layer when $L_{SI} \gg L_{Da}$, bulk effects dominate, when $L_{SI} < L_{Da}$ both contact and bulk effects are important. We will consider both cases, but L_{SI} will always be taken larger than both L_S and w where space charge effects prevail. For high applied voltages, injection through the forward biased contact becomes important and one carrier, trap modulated space charge current, control the charge transport. Both one carrier and double injection bulk phenomena have been studied by Lampert and Mark [6].

Fig. 1 gives the physical and electrical parameters of the structures. The doping of the N (P) contacts, having thicknesses L_N (L_P) of the order of a few μm , is large enough: N_D , (N_A) $\geq 10^{16} \text{ cm}^{-3}$, for the contact doping to have no significant effect on the results obtained.

2. Physical model: time independent drift–diffusion equations

Numerical solutions for electrons and holes transport across the structure were obtained using the drift–diffusion phenomenological (1D) model of conduction: Poisson’s equation, current equations and the continuity equations for electrons and holes. The space charge $\rho(x)$ is given by

$$\rho(x) = e[p(x) - n(x) + N_D - N_A + p_t - n_r] \quad (4)$$

p_t and n_r are the concentration of ionized deep donor or deep acceptor centers (we will consider either a deep donor or a deep acceptor) and N_D and N_A are the donor and acceptor densities assumed to be completely ionized ($T = 300 \text{ K}$). The conduction currents J_n and J_p are the sum of a drift and diffusion current and for steady state conditions, the continuity equations can be written:

$$\frac{1}{e} \frac{dJ_n}{dx} = U = - \frac{1}{e} \frac{dJ_p}{dx} \quad (5)$$

where U , the net Shockley–Read–Hall recombination rate, is for a deep donor:

$$U = \frac{np - n_i^2}{\tau_{nt}(p + p_{1t}) + \tau_{pt}(n + n_{1t})} \quad (6)$$

with: $n_e p_e = n_{1t} p_{1t} = n_i^2$. The relations between the capture cross sections σ_{nt} , σ_{pt} (cm^2), $v_{th,n}$ and $v_{th,p}$ the thermal velocities of the free electrons and holes and the minority carrier lifetime τ_{nt} , τ_{pt} are

$$\tau_{nt} = \frac{1}{N_t < \sigma_{nt} v_{th,n} >}; \quad \tau_{pt} = \frac{1}{N_t < \sigma_{pt} v_{th,p} >}; \quad \frac{\tau_{nt}}{\tau_{pt}} \approx \frac{\sigma_{pt}}{\sigma_{nt}} \quad (7)$$

An equivalent relation can be written for a deep acceptor, using n_{1r} , p_{1r} , τ_{nr} and τ_{pr} in Eq. (6).

The numerical modelisation is made at room temperature. Numerical solutions are obtained using a coupled method of resolution with an iterative algorithm of the Newton–Raphson type [7,8].

It is well established that EL2 is a deep donor with $\sigma_{nt} > \sigma_{pt}$ and the electron capture cross section is an increasing function of the electric field. Since we are interested in this work with low and intermediate applied voltage range, the capture cross sections and the mobilities are considered to be independent of the electric field E . The electron lifetime τ_{nt} has values in the range $10^{-7} - 10^{-10} \text{ s}$ [9–11]. On the other hand, the existence of hole traps in GaAs is mentioned but more problematic. Their densities and capture cross sections are not well known [2].

At thermal equilibrium outside the contact space charge region, assuming space charge neutrality with n_e , $p_e \ll p_{te}$, N_A where p_{te} is the equilibrium density of ionized deep centers in the bulk of the SI layer, we have

$$p_{te} \approx N_A \quad (8)$$

And:

$$n_e \approx n_{1t} \left[\frac{N_t}{N_A} - 1 \right] \quad \text{and} \quad p_e \approx p_{1t} \left[\frac{N_t}{N_A} - 1 \right]^{-1} \quad (9)$$

Equivalent relations are obtained for a deep acceptor compensating a shallow donor. With $n_r \approx N_D$, we obtain $n_e \approx n_{1r} [(N_r/N_D) - 1]^{-1}$ and $p_e \approx p_{1r} [(N_r/N_D) - 1]$.

3. Theoretical model

3.1. Relation between free carrier densities across the SI layers

N-SI or P-SI junctions differ largely from P–N junctions as, unlike the case of extrinsic SC, both carrier densities are affected under non-equilibrium conditions. There are no equivalent

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