An Efficient Numerical Method to Solve the Time-Dependent Semiconductor Equations Including Trapped Charge

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Abstract

In recent years, the increasing interest for Thin-Film Transistor (TFTs) has made the modeling of semiconductor devices with localized states increasingly important. In transient conditions, the dynamic change of trapped charge must be properly accounted for and two continuity equations ought to be considered in addition to the standard semiconductor equations. We propose here a novel methodology to solve this problem without increasing the number of resulting equations, which takes advantage of the locality of the trapped-charge conservation equations. In this way, the solution is achieved without resorting to approximation in the description of the trap-states dynamics.

1. Introduction

In recent years increasing attention has been paid to the design, fabrication and electrical characterization of amorphous and polycrystalline-silicon thin film transistors, which are being used in active-matrix flat-panel displays as addressing devices. Hence a growing interest is now devoted to the modeling and simulation of such devices which, due to the presence of large, energy-distributed, bulk (or grain-boundary) states, pose a few challenging simulation problems. In steady-state conditions the charge trapped in the gap states may correctly be accounted for by redefining the generation or recombination rate (e.g., [1]). In transient conditions, in order to take the dynamic variation of trapped charge into account, two more continuity equations must be added to the system describing the transport in the semiconductor. Such additional equations turn out to be differential in time but purely algebraic in space; thanks to this, a suitable manipulation can be found such that the model is solved without increasing the number of equations with respect to the drift-diffusion one. This makes the implementation easy while maintaining the efficiency of the drift-diffusion scheme. It is worth adding that no approximations in the description of the trap-state dynamics are involved here; in fact, opposite to other approaches, no particular assumption on the features of the intra-gap transitions is made.

2. Theory and Implementation

Taking the time dependence of both free and trapped charge into account, the complete system of device equations in transient conditions turns out to be

$$-\operatorname{div}(\varepsilon_s \operatorname{grad}\varphi) = q(p - n + N_D^+ - N_A^- + p_t - n_t), \tag{1}$$

$$\frac{\partial n}{\partial t} - (1/q)\operatorname{div}\boldsymbol{J}_n = -U_n, \qquad \frac{\partial p}{\partial t} + (1/q)\operatorname{div}\boldsymbol{J}_p = -U_p, \tag{2}$$

$$\frac{\partial n_t}{\partial t} = -U_{nt}, \qquad \frac{\partial p_t}{\partial t} = -U_{pt}, \tag{3}$$

where n_t, p_t are the concentrations of trapped charge and the remaining symbols have the usual meaning. The current densities $\boldsymbol{J}_{nt}$, $\boldsymbol{J}_{pt}$ associated to the traps are set to zero owing to the negligible mobility of trapped carriers. The system (1,2,3) is made of 5 equations in the unknowns φ, n, p, n_t, p_t. As anticipated in the Introduction, the number of equations can be reduced to 3; it is shown below that this result is achieved without approximations by incorporating the two continuity equations (3) in a modified expression of the recombination formula. It is worth adding that, for the sake of generality, the donor and acceptor states are treated separately; the corresponding concentrations of states are indicated by N_{tD}, N_{tA}. Combining (2) and (3) and observing that $q\,\partial(n + n_t - p - p_t)/\partial t = \operatorname{div}(\boldsymbol{J}_n + \boldsymbol{J}_p)$ one obtains $U_n - \partial n_t/\partial t = U_p - \partial p_t/\partial t$ which, after straightforward manipulation, leads to two linear, first-order equations in n_t and p_t:

$$\frac{\partial n_t}{\partial t} + D_A n_t = N_{tA}(\alpha_{nA} n + e_{pA}), \qquad \frac{\partial p_t}{\partial t} + D_D p_t = N_{tD}(\alpha_{pD} p + e_{nD}). \tag{4}$$

In (4) it is $D_A = \alpha_{nA} n + \alpha_{pA} p + e_{nA} + e_{pA}$, $D_D = \alpha_{nD} n + \alpha_{pD} p + e_{nD} + e_{pD}$, while e_{nA}, e_{pA}, e_{nD}, e_{pD} are the emission probabilities and $\alpha_{nA} = \sigma_{nA} u_{th}$, $\alpha_{pA} = \sigma_{pA} u_{th}$, $\alpha_{nD} = \sigma_{nD} u_{th}$, $\alpha_{pD} = \sigma_{pD} u_{th}$. The time discretization of (4), implemented for instance using the Backward-Euler method and referring to the i^{th} node, yields

$$n_{ti} = \left[\frac{n_t^{old} + N_{tA}(\alpha_{nA} n + e_{pA})\Delta t}{1 + D_A \Delta t}\right]_i, \qquad p_{ti} = \left[\frac{p_t^{old} + N_{tD}(\alpha_{pD} p + e_{nD})\Delta t}{1 + D_D \Delta t}\right]_i. \tag{5}$$

Eqs. (5) could also be obtained by first integrating (4) analytically and then taking Δt small. One sees that n_{ti}, p_{ti} are decoupled from each other; in particular, n_{ti}^{old}, p_{ti}^{old} in (5) are the values of the trapped charge calculated and stored at the previous time step. Since the probability of direct band-to-band transition is negligibly small, the net recombination rate U_n is given only by the transition of electrons between the conduction band and the gap states; similarly, the net recombination rate U_p is given by the transitions of holes between the valence band and the gap states. It follows that U_n, U_p can be written as functions of n, p, n_t, p_t:

$$U_n = \alpha_{nA}(nN_{tA} - nn_t) + \alpha_{nD} n p_t + e_{nD}(p_t - N_{tD}) - e_{nA} n_t, \tag{6}$$

$$U_p = \alpha_{pD}(pN_{tD} - pp_t) + \alpha_{pA} p n_t + e_{pA}(n_t - N_{tA}) - e_{pD} p_t. \tag{7}$$

Eq. (5) is replaced into the discrete form of (6,7); the result is then used to calculate the RHS of (2) at the current iterate. As a consequence, Eqs. (1) and (2) thus modified are fully equivalent to the original system (1,2,3) but, on the other hand, retain the same discretization scheme as in the trap-free case. Since no simplifying assumption is introduced, all the possible transitions are considered in (1) and (2); among these, in particular, are the intra-gap transitions between acceptor and donor states, which are seldom considered in the literature.

3. Results

Numerical simulations have been carried out using a two-dimensional version of the device-analysis program HFIELDS, supplemented with the method described above. The turn-off transient of an n-p polycrystalline-silicon diode is shown by way of example. The diode is biased with a 1 ns linear voltage ramp starting at 10^{-7} s, which brings the anodic voltage from 1 to -3 V. The program accounts for the large number of defects in polycrystalline silicon (grain boundaries, intra-grain defects etc.) assuming the density of states in the semiconductor proposed in [2]: the states located in the lower half of the gap are donor-like while those located in the upper half are acceptor-like. The energy distribution of each set of donor-like (acceptor-like) states is approximated by the sum of two exponential functions. Following [3], the distribution of states is assumed uniform in space; this is of course irrelevant as far as the scheme proposed here is concerned. The current across the two contacts of the diode is shown in Fig. 1. The calculation has been carried out accounting for the displacement component of the current: the perfect balance of the currents indicates that the charge is correctly conserved by the transient analysis. The corner at $t = 1$ ns corresponds to the end of the ramp. As a comparison, the same simulation has been repeated using the steady-state expression of p_t and n_t in Poisson's equation (1) and the corresponding values of U_p, U_n in the continuity equations (2), that is, one of the commonly-accepted approximations at low trap concentrations; the result is shown in Fig. 2 (on a different time scale from Fig. 1) and demonstrates the importance of taking the dynamics of trapped charge into account. One sees in fact that the currents flowing through the two contacts begin to differ as soon as the voltage drop across the diode changes. This means that the total charge within the device is not conserved. The importance of trap dynamics is also evident from Fig. 3, where the current is calculated at the same contact using the full model (continuous line) and the approximation of Fig. 2 (dashed line). The full model exhibits an intermediate transient corresponding to the release of the trapped charge, which is instead missing in the approximate model. The latter, in fact, exhibits a much sharper peak due to the displacement current only.

4. Acknowledgements

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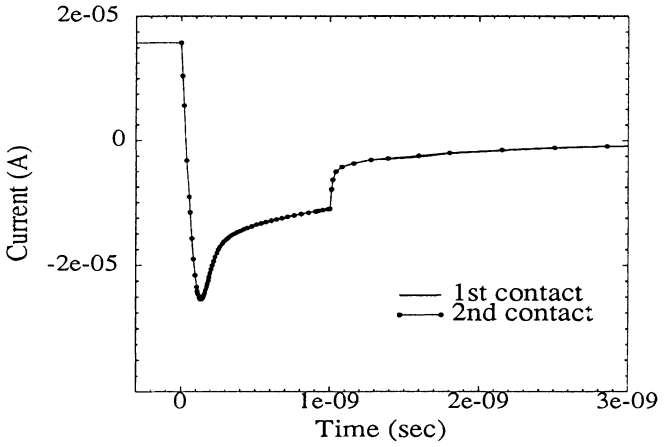

Fig. 1

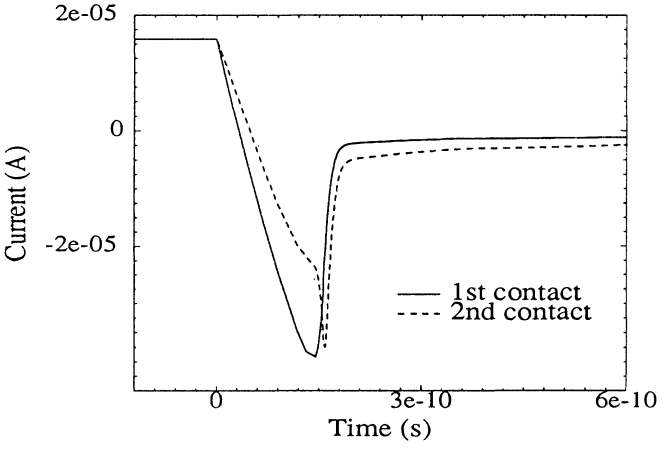

Fig. 2

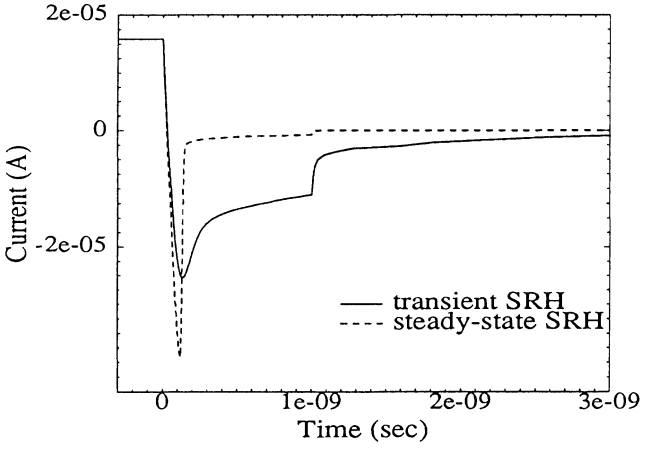

Fig. 3