A New Practical Method to Include Recombination-Generation Process in Self-Consistent Monte Carlo Device Simulation

Gyoyoung Jin, Edwin C. Kan and Robert W. Dutton
CISX 302, Stanford University, Stanford, CA 94305, USA
Phone: (415)725-6240, Fax: (415)725-7731, Email: gyjin@gloworm.stanford.edu

Introduction: A new practical method to incorporate recombination-generation (R-G) processes into self consistent Monte Carlo (MC) device simulation is considered. To calculate the R-G rate, a phenomenological expression like that for the well-known SRH mechanism is used instead of treating carriers in the microscopic interaction level. The most abundant and accurate information in MC simulation, carrier concentrations, can be utilized more directly to enhance the statistical stability and accuracy for the R-G effects. Realistic device examples, the minority carrier injection of a forward-biased n^+-p diode and the body effect from impact ionization of a 800 Å thin-film SOI MOSFET, are used to demonstrate the validity of this approach.

Past Work: In MC device simulation, many complicated physical models such as full-band structures and detailed scattering mechanisms can be incorporated into the calculations [1], but the R-G processes such as SRH and Auger have been usually neglected since they are very difficult to include computationally. However, the R-G processes are still very important for rigorous simulation, especially for devices whose behaviors are affected by both electrons and holes as in SOI MOSFET and bipolar devices. Even though rigorous microscopic models for the R-G processes have been proposed [2], there are still major difficulties arising from the large difference in time scales between the more frequent scattering events (e.g., electron-phonon scattering rates are usually larger than $10^{13}\mathrm{s}^{-1}$) and the R-G processes (less than $10^{9}\mathrm{s}^{-1}$). Therefore a new method is needed to reduce the statistical variation to achieve reasonable computational times.

The New Method: The SRH recombination is used as an illustration for the new method. Other R-G processes can be treated similarly. For rigorous simulation, both electrons and holes are simulated as particles and the Poisson equation is solved self-consistently on a time scale less than the inverse of the plasma frequency [3,4]. The numbers of electrons and holes that are recombined in the time interval δt within each mesh element can be estimated by

$$\delta N = \frac{n(t)p(t) - n_i^{\,2}}{\tau_n(n(t)+n_0) + \tau_p(p(t)+p_0)} Az\delta t \tag{1}$$

where A is the area of the mesh element and z is the effective element thickness. Notations n, p, n_i, n_0, p_0, τ_n and τ_p carry the usual meanings in the SRH expression. The Poisson equation is solved once within δt. If N_e and $N_e^{'}$ are the numbers of electrons in element A before and after the recombination, then $N_e^{'} = N_e - \delta N$. The recombination process can be accounted for by modifying the charge weightings of particels for electron in the mesh element

$$W_e^{'} = W_e \frac{N_e^{'}}{N_e} = W(1.0 - \frac{\delta N}{N_e}) \tag{2}$$

where W_e and $W_e^{'}$ are the charge weightings of electrons in element A before and after the recombination. Particles for holes are scaled by $(1.0 - \frac{\delta N}{N_h})$ to give the same number of recombined charges with the electrons in the mesh element, where N_h is the numbers of holes before recombination . In this new method, we are able to avoid the statistical process to distinguish any individual recombination event. Even though the probability for recombination during δt is very small since δt is on the order of $fsec$, the R-G effect based on (1) is still correctly reflected on the charge numbers. As an usual practice, when an MC simulation starts with an unphysical initial distribution, i.e. a carrier distribution obtained from drift-diffusion model, it is very difficult for microscopic R-G model to achieve steady state quickly. However if the number of carriers in each element is normalized according to a steady-state drift-diffusion model with (1) as the recombination term, steady state distributions can be reached on the order of the energy and momentum relaxation times. It is also possible to include the energy dependent recombination by using the energy-dependent recombination probability of each carrier in (1) [5]. For thermal generation, when δN in (1) is negative, an electron and a hole with the calculated charge weighting in (1) are added on the appropriate mesh elements with geometrically uniform distribution.

Device Examples: In Fig. 1, the carrier concentrations and recombination rate are shown for a simple n^+-p diode under a forward bias of $0.7V$. Rather short τ_n's and τ_p's such as 0.01, 0.1 and 0.5 ns are used to make the effects of recombination easily visible. Neutral and absorbing boundary conditions are used for both majority and minority carriers at contacts. Fig. 2 shows the carrier concentration, recombination rate and impact-ionized generation rate in an SOI MOSFET. The silicon layer is 800Å with $4 \times 10^{17} cm^{-3}$ acceptor doping, gate oxide is 70Å and $0.25\mu m$ long. Gate and drain are biased to 1.5 and 2.5 V, respectively. The recombination life time is 1.0 $nsec$ in the simulation. Although data collection time for recombination in Fig. 2(c) is 0.3 $psec$, we have a very stable recombination rate over the device. Detailed simulation results of device characteristics due to the R-G effects will be shown in the presentation.

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Reference:

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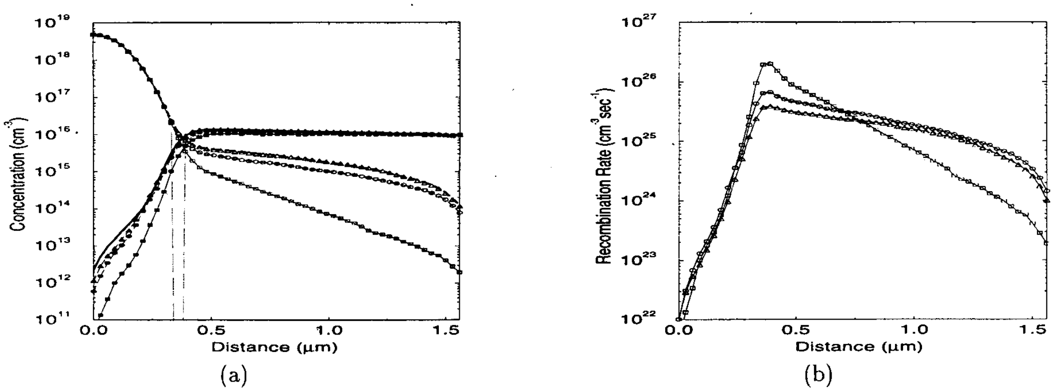

Fig. 1: In n^+-p diode, (a) electron (open symbols) and hole (solid symbols) concentrations and (b) recombination rates for τ = 0.1 (triangles), 0.05 (circles) and 0.01 (squares) *nsec*. Thick dashed and solid lines are for electron and hole concentations without the R-G model. The central dotted lines are for impurity profile with p-n junction at 0.36μm.

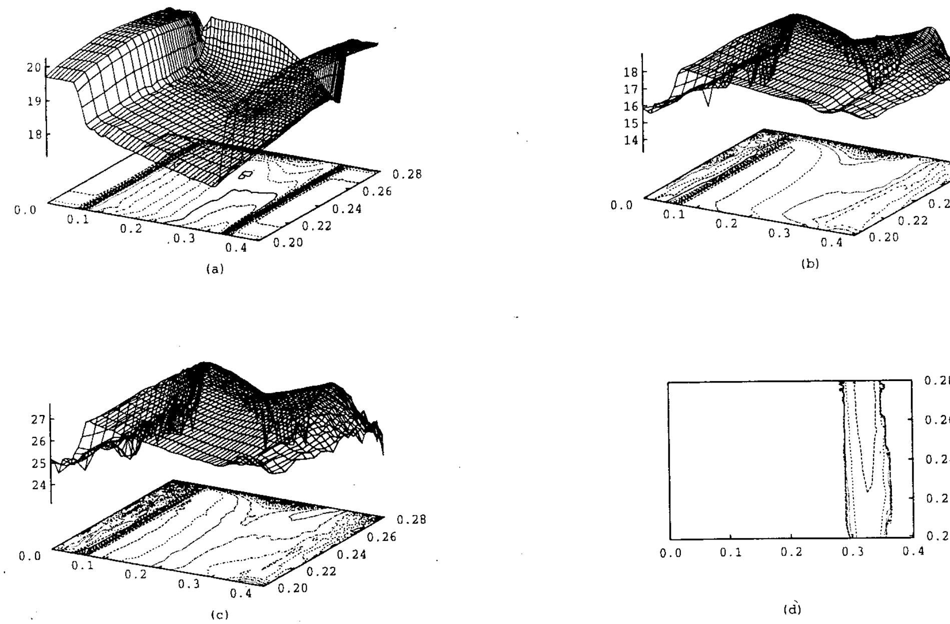

Fig. 2: In SOI MOSFET silicon layer; (a) electron (b) hole concentrations, (c) net recombination rate and (d) generation rate by impact ionization are shown in log_{10} scales. X and Y axes are in μm, electron and hole concentrations are in cm^{-3} and recombination/generation rates are in $cm^{-3}sec^{-1}$. Contour lines for generation rate are from 10^{24} to 10^{29} and spacing is 10 times.