

Monte Carlo algorithm for generation-recombination noise in semiconductors

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We present an original Monte Carlo procedure to account for generation-recombination noise through impurity centers in semiconductors. Numerical calculations are specialized to the case of holes in Si at 77 K. Results are found to compare favorably with available experiments.

An important source of noise specific for semiconductors comes from the statistical generation and recombination of charge carriers through impurity centers. This generation-recombination (GR) noise, being proportional to the square of the current flowing in a two-terminal network, generally yields an intrinsic limit to the performances of a device when increasing voltages are applied and/or submicron structures are considered. On the other hand, the microscopic interpretation of this type of noise can supply useful information concerning trapping and detrapping not available otherwise.

While several macroscopic approaches to GR noise can be found in the literature,¹ microscopic theories are very scarce. Furthermore, the concomitant presence of nonlinear effects in the applied field (hot-electron effects) makes a rigorous analytical approach to the problem very difficult.

We present here a novel Monte Carlo (MC) algorithm to calculate GR noise at a given electric field in nondegenerate semiconductors. The advantages of the MC procedure are that it provides an accurate microscopic description of the physical processes,² and it does not require any assumption on the carrier distribution function. The essence of the result is based on the interpretation of GR noise as a particular case of diffusion noise associated with two groups of carriers, one moving freely in the conduction band and the other trapped on the impurities³ (one impurity level is here considered). Under steady-state conditions and by neglecting $1/f$ noise and two-particle interaction, the spectral density S_I at low frequencies can be written as

$$S_I(\omega \rightarrow 0) = (4e^2 A N_I / L) D_{\text{tot}}, \quad (1)$$

with

$$D_{\text{tot}} = \int_0^\infty \overline{\delta v \delta v(t)} dt. \quad (2)$$

Here e is the electron charge, A the cross-sectional area of the sample, L its length, N_I the total concentration of impurities, $\delta v(t) = v(t) - v_d$ the carrier velocity fluctuation around the steady state value, and the bar denotes a time average. Equations (1) and (2) generalize Price's relationship⁴ when the velocity $v(t)$ of the carrier accounts for trapping and detrapping processes.

By introducing into a standard MC procedure GR processes as an additional scattering mechanism, the longitudinal D_{tot}^l and transverse D_{tot}^t components of D_{tot} can be cal-

culated at long times from their definition:

$$D_{\text{tot}}^l = \frac{1}{2} \frac{d}{dt} \overline{x^2 - \bar{x}^2}, \quad (3)$$

$$D_{\text{tot}}^t = \frac{1}{2} \frac{d}{dt} \overline{y^2}, \quad (4)$$

where x and y are the carrier positions parallel and perpendicular to the applied electric field E , respectively.

Theory is here specialized to the case of holes in Si. The microscopic model follows from Ref. 5. It uses a single valence band (the heavy one), warped with nonparabolic effects accounted for. Acoustic, nonpolar optical and ionized impurity scattering mechanisms are considered. A nonradiative GR mechanism is introduced using the results of Ref. 6. Accordingly, the probability per unit time of recombination $P_{\text{rec}}(\epsilon)$ is given by⁷

$$P_{\text{rec}}(\epsilon) = N_I \rho_{\text{eq}} u h(\epsilon), \quad (5)$$

where ρ_{eq} is the equilibrium recombination rate per unit volume, u is the fraction of ionized impurities, and

$$h(\epsilon) = l(\epsilon) / \langle l(\epsilon) \rangle_{\text{eq}}, \quad (6)$$

$$l(\epsilon) = \left(\frac{\xi}{\alpha} \right)^{1/2} \int_0^\infty \frac{(\xi + \eta)^2}{\xi} \times \left[\left(1 + \frac{1}{4} (\xi + \eta) \right)^2 - \xi \right]^{-3} \times \left[1 - \exp \left(- \frac{\xi + \eta}{\alpha} \right) \right] \times \left[1 - \left(1 + \frac{\eta}{\alpha} \right) \exp \left(- \frac{\eta}{\alpha} \right) \right] d\eta, \quad (7)$$

$$\alpha = 2KT/m^*s^2; \xi = 2\epsilon/m^*s^2. \quad (8)$$

Here $m^* = 0.53$ is the effective mass at the top of the band, $s = 6.53 \times 10^5$ cm/s is an average sound velocity, K the Boltzmann constant, T the lattice temperature, and $\langle \rangle_{\text{eq}}$ denotes average over the equilibrium distribution function.

The MC technique requires the evaluation of the probability per unit time of generation from an impurity state to a given energy in the valence band $P_{\text{gen}}(\epsilon)$. By using the equilibrium detailed balance for GR processes we obtain

$$P_{\text{gen}}(\epsilon) = \frac{2}{\sqrt{\pi}} \gamma \exp \left(- \frac{\epsilon}{KT} \right) \left(\frac{\epsilon}{KT} \right)^{1/2} h(\epsilon), \quad (9)$$

where γ is the generation rate. In the single carrier simula-

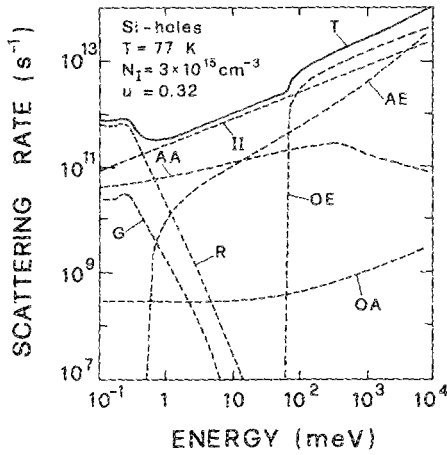


FIG. 1. Scattering rates as a function of energy for holes in Si at 77 K with $N_T = 3 \times 10^{15} \text{ cm}^{-3}$. Symbols have the following meaning: AA (acoustic absorption), AE (acoustic emission), OA (optical absorption), OE (optical emission), II (ionized impurity), G (generation), R (recombination), T (total).

tion, when a recombination process occurs, a trapping time is determined exponentially distributed according to γ . Then, a generation process follows immediately, in which the final energy of the carrier in the valence band is stochastically assigned through Eq. (9). Under steady-state conditions, the ratio between the total time spent in the valence band and the total time of the simulation represents the fraction of ionized impurities u .

Calculations have been performed at 77 K for an acceptor concentration (boron) $N_T = 3 \times 10^{15} \text{ cm}^{-3}$ (room-temperature resistivity = $4.8 \Omega \text{ cm}$). As input parameter for the GR scattering probabilities we take $\rho_{\text{eq}} = 4.2 \times 10^{-6} \text{ cm}^3/\text{s}$, as determined for the case of boron in Si in Ref. 5. Then a value of γ equal to $1.9 \times 10^9 \text{ s}^{-1}$ is obtained from the balance equation for GR rate at equilibrium:

$$N_T \rho_{\text{eq}} u_{\text{eq}}^2 = \gamma(1 - u_{\text{eq}}), \quad (10)$$

where u_{eq} is taken equal to 0.32 from statistical calculations. Let us emphasize that the choice for the GR parameters is in good agreement with available experiments.⁸

Figure 1 shows the different scattering probabilities per unit time used in the MC simulation. We notice that recombination is the dominant process at energies below 1 meV. Therefore, a precise knowledge of the distribution function in the low-energy tail is needed in order to obtain reliable results.

The dependence with electric field of D_{tot} is reported in Fig. 2. Here D_{tot}^I is found to initially increase with the electric field strength, reach a maximum, and finally decrease. This behavior can be interpreted by decomposing D_{tot}^I into its three contributions⁹:

$$D_{\text{tot}}^I = u D_{\text{vf}}^I + D_{\text{gr}} + D_{\text{cross}}, \quad (11)$$

D_{vf}^I (responsible of Johnson-Nyquist noise) is the diffusion coefficient associated with velocity fluctuations of the carriers in the absence of GR mechanisms. D_{gr} (responsible of GR noise) is the diffusion coefficient due to carrier density fluctuations, and D_{cross} is the diffusion coefficient originated by the cross correlations between velocity and density fluctuations.

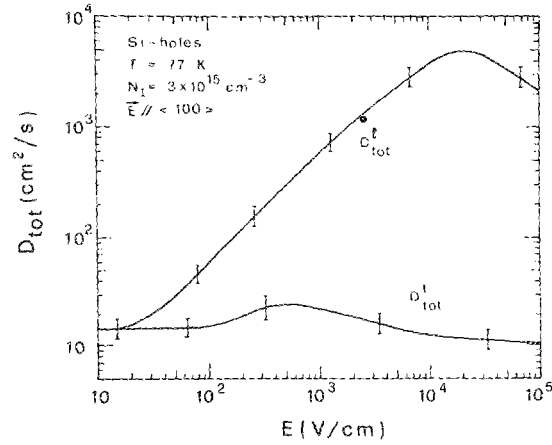


FIG. 2. Diffusivity as a function of the electric field strength for the case of holes in Si at 77 K. Curves report Monte Carlo calculations with bars indicating uncertainties. The point represents the only experimental result available at present (see Ref. 8).

tuations. D_{gr} and D_{cross} are respectively proportional to v_d^2 and v_d . Thus, they vanish at equilibrium, while at increasing electric field strengths they are responsible for the large values of D_{tot}^I . At the highest fields, due to carrier heating v_d tends to saturate and all impurities to be ionized ($u \rightarrow 1$). As a consequence D_{tot}^I finally decreases. D_{tot}^0 , having neither GR nor cross-correlation contribution, behaves as the thermal transverse diffusion coefficient in absence of GR mechanisms, scaled by the factor u . Its wavy behavior reflects the different role played by the ionized impurity scattering at increasing electric fields. A remarkable agreement with the only experiment available at present is also evidenced by Fig. 2.

For completeness, in Fig. 3 we report the dependence upon the electric field strength of the fraction of ionized impurity $u(E)$ and of the carriers lifetime $\tau(E) = u/[\gamma(2 - u)]$ (Ref. 1) as obtained from the simulation. Both quantities exhibit a systematic increase with electric field strength due to carrier heating.

In conclusion, a novel Monte Carlo algorithm is presented to calculate the spectral density of current fluctuations in the presence of Johnson-Nyquist as well as genera-

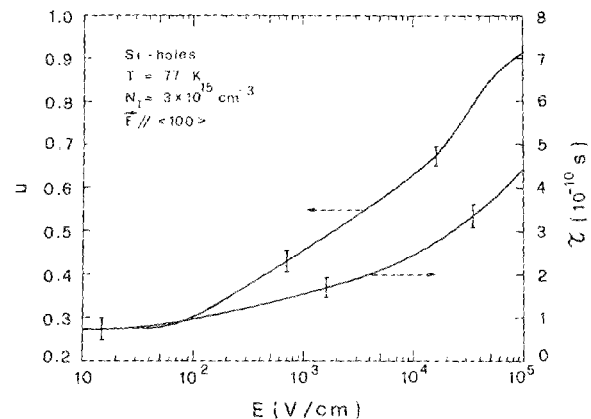


FIG. 3. Fraction of ionized impurities (left scale) and generation-recombination lifetime (right scale) as a function of electric field for holes in Si at 77 K. The error bars indicate the uncertainty of the Monte Carlo results.

tion-recombination noise sources. Theory does not contain any arbitrary parameter since the physical quantities of interest are provided by independent experiments. Furthermore, the dependence of γ upon the electric field (Poole-Frenkel effect) can be easily accounted for if necessary.

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