Nonexponential generation-recombination dynamics in doped semiconductors as a possible source of high-frequency $1/f$ noise

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(Received 9 February 1993)

We present a theoretical study of generation-recombination processes from shallow impurities which includes self-consistently the contribution of the impurity excited levels. Making use of an original Monte Carlo simulation which accounts for both the kinetic energy of the carrier and its potential energy near the impurity, we have solved the semiclassical Boltzmann equation to investigate the dynamics of generation-recombination processes on a kinetic level. Calculations performed for the case of p-type Si clearly evidence a nonexponential distribution of the microscopic times spent by the carriers in the impurity centers and in the conducting band. This in turn leads to the impossibility of a rigorous definition of a carrier lifetime and therefore to a possible source of high-frequency $1/f$ noise. The theory is found to compare favorably with available experiments.

I. INTRODUCTION

An important source of noise in doped semiconductors stems from the processes of capture and release of carriers from shallow-impurity levels: the so-called generation-recombination (GR) noise. The theoretical treatment of this noise is based on a mesoscopic approach which, in the simple case of a two-level system (e.g., conducting band and impurity levels), requires two parameters: namely, the variance of the carrier number fluctuations and the carrier lifetime.[1,2] Rigorously, a lifetime should correspond to an exponential distribution of both the microscopic times spent by the carriers in the conducting band and in the impurity centers. However, such a simple distribution is expected to be strongly modified by the presence of a large number of excited levels where the carriers can spend some time and then come back to the conducting band without visiting the ground state. The possibility of a nonexponential kinetics of generation-recombination processes has been recently investigated experimentally for the case of ultrafast recombination of holes with shallow acceptors by means of picosecond infrared spectroscopy.[3] The case of GR noise in the presence of excited states of an impurity trapping center was also treated briefly by Van Vliet;[4] however, in that treatment instantaneous quasiequilibrium between the excited states and the ground state was assumed, which is not justified by the present study. Furthermore, the theoretical analysis of the recombination process assisted by acoustic phonons is based on the cascade-capture model which requires the knowledge of the so-called "sticking function," defined as the probability of a carrier reaching the ground state of the impurity levels without coming back to the conducting band.[5–9] Such an analysis takes into account the effect of the excited impurity levels only indirectly, in spite of its recognized importance in determining the dynamics of GR processes.[10,11]

To avoid the above limitations, in this paper we use an original Monte Carlo (MC) simulation, which extends the semiclassical Boltzmann equation to treat GR processes at impurity centers. The scheme includes both the kinetic energy of the carrier and the potential energy of the impurity thus providing a microscopic calculation of the times spent by the carriers in the conducting band and in the impurity levels, as well as of the correlation function of the fluctuations of the number of free carriers and its associated spectral density. This enables us to investigate the limits of validity and deviations from existing theories.

The paper is organized as follows. Section II presents the theoretical model for the analysis of the correlation function of the fluctuations of the number of free carriers and its associated noise spectral density. The Monte Carlo procedure is briefly described in Sec. III. Section IV reports the results of the simulations. Finally, the main conclusions are drawn in Sec. V.

II. THEORETICAL MODEL

The primary quantity which describes electronic noise is the spectral density of current fluctuations $S_I(f)$. It

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can be measured more or less directly in different ranges of the frequency f and microscopically interpreted from the calculation of its theoretical counterpart, which is the associated correlation function $C_I(t)$. As a matter of fact, the relationship between the above two quantities is given by the Wiener-Khintchine theorem,[12] which states that

$$S_I(f)=2\int_{-\infty}^{+\infty}\exp(i2\pi ft)C_I(t)dt\ , \tag{1}$$

$$C_I(t)=\overline{\delta I(0)\delta I(t)}\ , \tag{2}$$

where $\delta I(t)=I(t)-\bar{I}$ is the total current fluctuation around the average value $\bar{I}$, and the bar denotes time average. This methodology has recently led to the development of a noise spectroscopy which has proven to be very fruitful for investigating the transport properties of materials and devices.[13–18]

At equilibrium, one of the most important properties is that the spectral density remains frequency independent (white noise) up to values comparable to the momentum relaxation rate of the carrier ensemble. Under the application of an external electric field, when quadratic effects in the current become important, deviations from the simple white spectrum occur and excess noise contributions (so called because of their explicit dependence on the net current flow) can be detected.[12] It should be noticed that the fluctuations responsible for excess noise are often present also at equilibrium; in the current noise, however, they manifest themselves only under nonequilibrium situations. Nevertheless, from a theoretical point of view these contributions can be calculated also at equilibrium (which is the case of the present paper). In this context, the presence of a low-frequency $1/f$ contribution (also called flicker noise) has been found to be a common feature of excess noise, the origin of which remains still controversial.[19–23]

For a homogeneous sample where the transport of charge carriers occurs on the basis of a two-level model (i.e., the conducting band and an impurity level which supplies the carriers) and neglecting cross correlations $C_I(t)$ is expressed as[18]

$$C_I(t)=\frac{e^2}{L^2}\bar{N}^2\overline{\delta v_d(0)\delta v_d(t)}+\bar{I}^2\frac{\overline{\delta N(0)\delta N(t)}}{\bar{N}^2}\ , \tag{3}$$

where e is the absolute value of the electron charge, L is the length of the sample, N is the number of free carriers, v_d is the free-carrier drift velocity, and I is the current flowing in the outside circuit. The two terms on the right-hand side of Eq. (3) are responsible for thermal and excess (in this case GR) noise contributions, respectively.

Hereafter we will focus only on the GR contribution, i.e., the second term on the right-hand side of Eq. (3). By Fourier transforming this term, we obtain the following expression for the associated current spectral density S_{Igr}:

$$S_{Igr}(f)=\frac{2\bar{I}^2}{\bar{N}^2}\int_{-\infty}^{\infty}\exp(i2\pi ft)\overline{\delta N(0)\delta N(t)}dt\ . \tag{4}$$

The calculation of the above spectral density is considerably simplified for the case of noninteracting particles. Here particle-particle interaction not only means a direct scattering between two carriers, but also a correlation introduced by the occupancy factor of the impurity levels. Thus, for a single-particle simulation only a linear recombination can be treated. (This may give a small error in the noise magnitude due to neglecting the bimolecular transition statistics.[24]) For this purpose, we make use of the following property:[14,18]

$$\overline{\delta N(0)\delta N(t)}=N_I\overline{\delta u(0)\delta u(t)}=N_I C_u(t)\ , \tag{5}$$

where N_I is the total number of carriers inside the sample participating in the transport here assumed to be constant at any time, $\delta u(t)=u(t)-\bar{u}$, $u(t)$ being the random telegraph signal due to the state of the carrier:

$$u(t)=\begin{cases}1 & \text{if carrier is free}\\ 0 & \text{if carrier is trapped}\ ,\end{cases} \tag{6}$$

and $\bar{u}$ is the average value of $u(t)$ which gives also the average fraction of free carriers $\bar{N}/N_I$. Thus, for the case of noninteracting particles, Eq. (4) reduces to

$$S_{Igr}(f)=\frac{2\bar{I}^2}{\bar{u}^2N_I}\int_{-\infty}^{+\infty}\exp(i2\pi ft)C_u(t)dt\ . \tag{7}$$

The initial values of $C_u(t)$ can be exactly calculated since by construction it is $\overline{u^2}=\bar{u}$. Therefore, we obtain

$$C_u(0)=\overline{\delta u(0)^2}=\bar{u}(1-\bar{u})\ . \tag{8}$$

Concerning the time behavior, within a relaxation-time approximation, it is[2]

$$C_u(t)=C_u(0)\exp(-t/\tau_l)\ , \tag{9}$$

where $C_u(0)$ is given by Eq. (8) and τ_l is the carrier lifetime. For GR processes governed by linear kinetics it is[2,12]

$$\tau_g=\frac{1}{\gamma}\ , \tag{10a}$$

$$\tau_r=\frac{\bar{u}}{\gamma(1-\bar{u})}\ , \tag{10b}$$

$$\tau_l=\left[\frac{1}{\tau_g}+\frac{1}{\tau_r}\right]^{-1}=\frac{\bar{u}}{\gamma}\ , \tag{10c}$$

where γ is the equilibrium generation rate, τ_g is the generation time, and τ_r is the average (over the energy distribution function) recombination time. In the above derivation, both generation and recombination times are assumed to be exponentially distributed. Equations (9) and (10) imply Lorentzian noise spectra with a corner frequency corresponding to the fluctuator lifetime. In general, the presence of more fluctuators with a distribution of lifetimes over many orders of magnitude can lead to more complicated spectra and, under suitable conditions, to a $1/f$ behavior.[12,19–22] However, in general, the microscopic times of GR processes might not be exponentially distributed, which leads to deviations from the simple approximations of Eqs. (9) and (10) and, therefore, of the standard Lorentzian spectrum. This will be investigated in the following section.

III. MONTE CARLO SIMULATION

The theoretical approach used most to treat GR processes in semiconductors is the cascade-capture model, originally introduced by Lax[5] and further elaborated by the Leningrad group.[6,7] Within Lax's approach, because of the use of the sticking function, whose determination remains a complicated affair,[10,25–27] the effect of excited impurity levels during recombination remains hidden in spite of its recognized importance in determining the dynamics of recombination[11] and low-temperature breakdown phenomena.[28] On the other hand, the Leningrad group[6,7] has treated the problem at a phenomenological level by using an energy-relaxation-time approximation to solve the appropriate kinetic equation.

Here we make use of the MC technique for the microscopic calculation of $C_u(t)$ which is based on a simulation of the carrier motion in the total-energy space, where we assume that the positive-energy region corresponds to conducting states while the negative-energy region corresponds to bound states. We consider randomly distributed impurities and all transitions are assumed to occur instantaneously in space and time; in particular, transitions in the negative-energy region supposedly are to occur at the impurity site. The mechanism responsible for GR processes is taken to be the cascade-capture model assisted by acoustic modes. Accordingly, due to acoustic-phonon emission a carrier can enter the negative-energy region, where it has two possibilities: to spend some time in the excited levels and then come back to the conducting band, or to penetrate deeply into the negative-energy region thus being finally captured to the impurity center. When the latter possibility occurs we stop the simulation and generate a new carrier in the conducting band with a velocity determined from detailed balance because we do not take into account the capture on the ground state. We notice that, being a simulation of the carrier motion in the energy-configuration space of an impurity center, it resembles a molecular-dynamics calculation.

More details of the microscopic model can be found in Ref. 29. Here we want to point out that the semiclassical approach (Boltzmann equation) can be applied in the whole energy region covering the conducting and the bound states up to $K_B T < E_I^{(1)}$, where $E_I^{(1)}$ is the energy of the first ionized level.[7] The above scheme is applied to the case of p-type silicon at equilibrium at temperatures below 77 K so that the above condition is fulfilled. A single spherical band model, the heavy holes, with a temperature-dependent effective mass m_h which accounts for nonparabolic effects, is used.[30] The scattering rates have been evaluated as a function of the carrier total energy by making a space average over the volume belonging to one impurity, showing a tail in the negative-energy region due to the presence of the impurities.[6,29] In particular, in our self-consistent treatment the transition to the negative-energy region occurs at the energy level associated with the fluctuational Coulomb potential of the impurity;[6] however, the Coulomb potential for a single impurity should be cut off at the percolation energy value,[10] which leads to a somewhat larger volume average than in our case and can slightly modify the calculation of the scattering rates. We notice that, being at equilibrium, we need to follow only changes of the total energy due to scatterings, and elastic-scattering mechanisms, such as impurity scattering, can be neglected.

We remark that the physical plausibility of the above scheme has been checked through a first-principle calculation of the recombination cross section assisted by acoustic phonons at shallow impurities.[29,31]

IV. RESULTS

From the analysis of the random telegraph signal $u(t)$ we have calculated the histograms of the number of recombinations N_R [i.e., times with $u_i(t)=1$], and of generations N_G [i.e., times with $u_i(t)=0$] associated with a given time interval. The histograms of N_R for different impurity concentrations are shown in Fig. 1. The distribution of N_R exhibits a double exponential decay, one with a short characteristic time ($\simeq 8\times 10^{-11}$ s), which is independent of the impurity concentration, and the other with a long characteristic time which decreases with increasing concentration. The fact that most of the recombinations occur at short times is attributed to the strong coupling between GR processes and scattering mechanisms, which occurs in the lowest-energy region of the carrier energy distribution function. Hence, when a carrier undergoes a transition from the negative- to the positive-energy region it has a great probability of recombining before having visited all the accessible regions of the positive-energy distribution function. Therefore, the carrier, due to the energy dependence of the scattering rates, can keep the memory of the generation process up to the next recombination, in contrast to the case when, once generated, it scatters many times in the conducting band, thus losing the memory of GR processes.

The short-time decay is independent of the acceptor concentration, but it depends on the temperature. In Fig. 2 we have reported the time associated with the short-time decay of the distribution of the recombination times

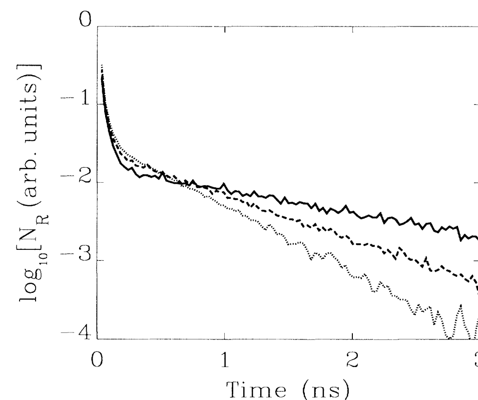

FIG. 1. Histogram of the number of recombinations N_R as a function of the time spent by the simulated carrier in the positive-energy region at $T=77$ K. The continuous, dashed, and dotted lines refer to the results obtained from the Monte Carlo simulation of p-Si at equilibrium with, respectively, $N_A=4\times 10^{14}$, 3×10^{15}, and 1×10^{16} cm^{-3}.

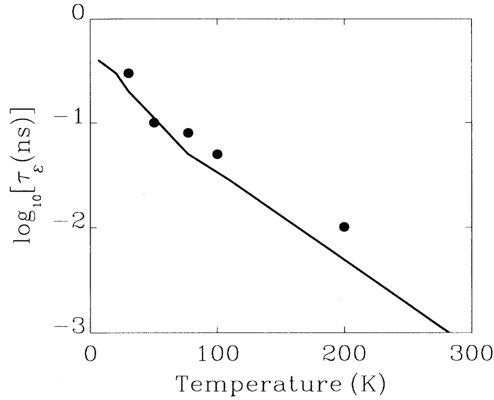

FIG. 2. Energy relaxation time τ_ϵ as a function of the temperature. The line represents the result determined through Eq. (11) of the text and the symbols represent the Monte Carlo results of p-Si at equilibrium obtained from the short-time decay of the distribution of the recombination times.

as a function of the temperature. It can be noticed that the results are in good agreement with the energy relaxation time determined by the balance equation

$$\tau_\epsilon = \frac{\bar{\epsilon} - \frac{3}{2} K_B T}{e \bar{v}_d E} , \tag{11}$$

where $\bar{\epsilon}$ is the average carrier energy, K_B is the Boltzmann constant, T is the lattice temperature, and E is the electric field.

Concerning the long-time decay of the distribution of the recombination times, we have found that it is independent of the temperature, but it decreases with increasing acceptor concentration N_A. This result is shown in Fig. 3. Finally, we conclude that due to the nonexponential distribution of the recombination times, it is not possible to introduce a rigorous definition of a recombination time τ_r.

Now we discuss the distribution of the generation times. In Fig. 4(a) the time histogram of the times spent by the carriers on the impurity levels at 77 K is shown for different acceptor concentrations. Here we cannot identify any exponential decay related to a characteristic generation time τ_g; rather, a broad distribution of characteristic times is required to describe these histograms. This behavior is attributed to the presence of a large number of impurity excited levels. Furthermore, the fact that the distribution is independent of the acceptor concentration confirms that, for a nondegenerate system where there is always a large number of accessible states in the conducting band, the generation frequency at equilibrium is an intrinsic property of the trap being independent of the acceptor concentration. In Fig. 4(b) the histogram of the times spent by the carriers on the impurity levels is shown for an acceptor concentration $N_A = 3\times 10^{15}$ cm^{-3} and for different temperatures. Also in this case a nonexponential shape of the above distribution is found; it can be noticed that long generation times are privileged at decreasing temperatures. This is due to the fact that at low temperatures the probability of phonon emission in the negative-energy region is always larger than the absorption probability.[29] As a conse-

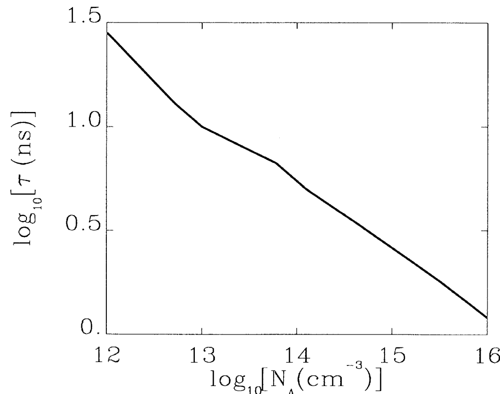

FIG. 3. Long-time decay of the distribution of the recombination times as a function of the acceptor concentration obtained from the Monte Carlo simulation of p-Si at equilibrium.

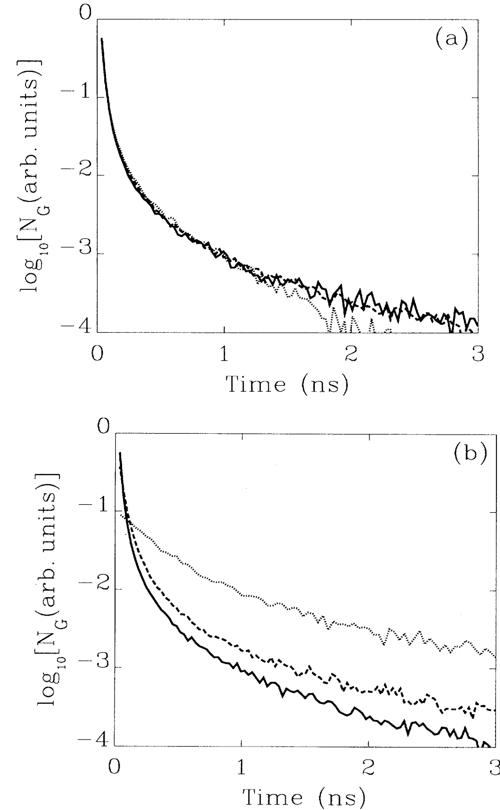

FIG. 4 Histogram of the number of generations N_G as a function of the time spent in the negative-energy region obtained from the Monte Carlo simulation of p-Si at equilibrium. (a) refers to $T = 77$ K and the continuous, dashed, and dotted lines refer, respectively, to $N_A = 4\times 10^{14}$, 3×10^{15}, and 1×10^{16} cm^{-3}. (b) refers to $N_A = 3\times 10^{15}$ cm^{-3} and the continuous, dashed, and dotted lines refer, respectively, to $T = 77$, 50, and 10 K.

quence, a carrier spends most of the time trapped on the impurity levels and the time distribution shifts to longer values.

The above considerations lead to the impossibility of providing a kinetic calculation of the lifetime τ_l, which has been defined in Eq. (10c). Therefore, we can expect deviations from the simple relaxation form of $C_u(t)$ as given in Eq. (9). This is shown in Fig. 5, where the normalized autocorrelation function $C_u(t)/C_u(0)$ is found to exhibit a nonexponential behavior in all the cases which we have considered. In particular, from Fig. 5(a) it can be noticed that by increasing the acceptor concentration, the autocorrelation function decays faster. This behavior reflects the decreasing of the longest times in the distribution of the recombination times at increasing acceptor concentrations, as shown in Fig. 1. In Fig. 5(b) we have reported the autocorrelation function for a given acceptor concentration at different temperatures. It can be noticed that the nonexponential decay is confirmed at all the temperatures. Furthermore, going from 77 to 50 K the autocorrelation function exhibits a slower time decay, while no further change is observed in going from 50 to 10 K. This is because below 50 K, GR processes are practically determined by the recombination mechanism only, being the shortest one and independent of the temperature.

As a consequence of the nonexponential behavior of the above correlation functions, the associated spectral densities $S_u(f)$ deviate from the usual Lorentzian shape, showing, in particular, a nearly $1/f$ dependence in the frequency range $10^8 < f < 10^{10}$ Hz at 77 K (see Fig. 6).

Theoretical calculations are compared with experimental results in Fig. 7. Here, the current spectral density at low frequency associated with GR noise is reported as a function of the current flowing in the sample. Experimental data are extrapolated from a set of experiments of the Montpellier group[17] by subtracting from the total spectral density the contribution of Nyquist noise. Theoretical values are obtained by using Eq. (7) where the correlation function $C_u(t)$ and the value of $\bar{u}$ have been calculated from the Monte Carlo simulation, while

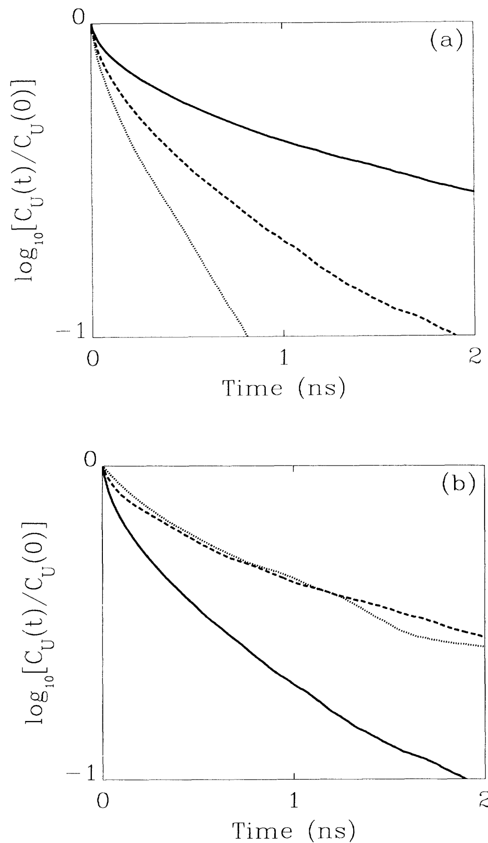

FIG. 5. Autocorrelation functions of the fluctuations of the number of free carriers normalized to their initial values obtained from the Monte Carlo simulation of p-Si at equilibrium. (a) refers to $T=77$ K and the continuous, dashed, and dotted lines refer, respectively, to $N_A=4\times10^{14}$, 3×10^{15}, and 1×10^{16} cm^{-3}. (b) refers to $N_A=3\times10^{15}$ cm^{-3} and the continuous, dashed, and dotted lines refer, respectively, to $T=77$, 50, and 10 K.

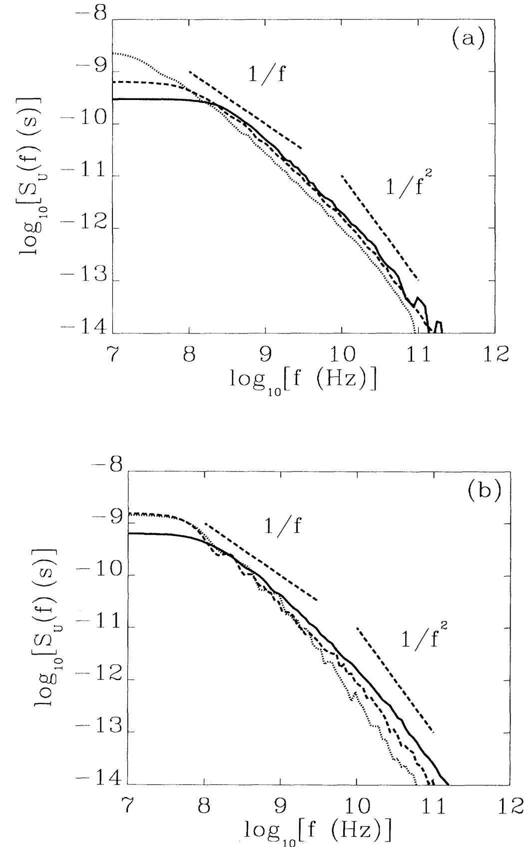

FIG. 6. Spectral density associated with the fluctuations of the number of free carriers obtained from the Monte Carlo simulation of p-Si at equilibrium. Together with the spectral densities, the behaviors $1/f$ and $1/f^2$ are shown as guides for the eyes. (a) refers to $T=77$ K and the continuous, dashed, and dotted lines refer, respectively, to $N_A=4\times10^{14}$, 3×10^{15}, and 1×10^{16} cm^{-3}. (b) refers to $N_A=3\times10^{15}$ cm^{-3} and the continuous, dashed, and dotted lines refer, respectively, to $T=77$, 50, and 10 K.

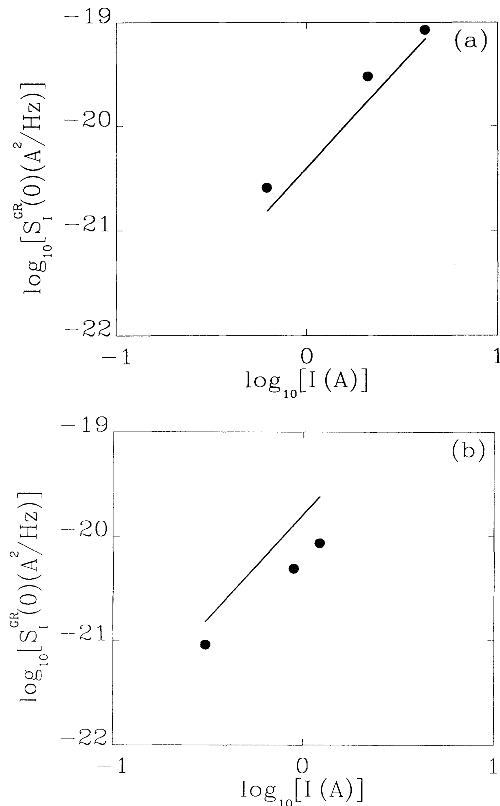

FIG. 7. Low-frequency spectral density of current fluctuations associated with generation-recombination processes as a function of the current in *p*-Si at 77 K with $N_A = 3\times10^{15}$ cm^{-3} (a) and $N_A = 4\times10^{14}$ cm^{-3} (b). The symbols refer to the experimental results deduced from Ref. 17 and the line represents the theoretical results obtained from the Monte Carlo simulation.

the value of N_I has been chosen consistently with the sample geometry (see Ref. 17). We recall that the simulation has been performed at equilibrium and, therefore, the possible dependence of $C_u(t)$ and $\bar{u}$ on the current has been neglected: in other words, hot-carrier effects have been disregarded. The agreement between the theory and the experiments is off by at most a factor 2. In view of the lack of arbitrary parameters to force the fitting, such an agreement is considered to be satisfactory thus confirming the physical plausibility of the model used.

V. CONCLUSIONS

We present a Monte Carlo simulation of generation-recombination processes at shallow-impurity centers accounting for the presence of a large number of excited levels. Calculations clearly demonstrate a nonexponential distribution of both the recombination and generation times associated with capture and release of charge carriers from impurity centers at equilibrium. The former distribution is discussed in terms of the coupling between relaxation in number of free carriers and in their energy, while the latter is attributed to the presence of a large number of impurity excited levels. As a consequence, GR processes cannot be described by a single lifetime, rather a distribution of characteristic times is required and the autocorrelation function of the fluctuations of the number of free carriers strongly deviates from a simple exponential decay. This, in turn, leads to significant deviations of the correspondent spectral density from the standard Lorentzian shape. Results for the case of acceptors in Si give evidence of a nearly $1/f$ type of spectrum in the region of high frequencies centered around 1 GHz. This behavior extends over two decades before flattening in the low-frequency region where an appropriate comparison with the experiments of the Montpellier group shows a satisfactory agreement.

ACKNOWLEDGMENTS

This work has been partially supported by the Consiglio Nazionale delle Ricerche (CNR) and CEC ESPRIT II BRA 3017 project.

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