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Coupled-Langevin-equation analysis of hot-carrier transport in semiconductors

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Using the results of a Monte Carlo simulation, a set of coupled Langevin equations for the relevant variables: the fraction of free carriers, the velocity, and energy, is constructed and applied to the case of *p*-type Si at 77 K under the influence of an electric field of arbitrary strength. The properties of the Langevin equations, by separating the terms associated with dissipation from those associated with fluctuations, is found to help the physical understanding of the results. The relaxation and generalized-diffusion matrices describing dissipation and fluctuations, respectively, are evaluated for different free-carrier concentrations. Their physical interpretation is shown to describe the cross correlation among different variables, which is present at equilibrium or is induced by the field.

I. INTRODUCTION

The concept of a Langevin equation has been originally introduced to study the Brownian motion of a particle coupled to a heat bath with large number of degrees of freedom. Since then it has been successfully applied to many fields where stochastic processes are important.[1,2] The main reason of its importance lies in the decoupling of the damping forces from those leading to fluctuations which, although both are caused by the same microscopic processes, helps the intuitive understanding of the physics involved. If one is interested in first-order transport quantities (i.e., mean values), only the dissipative part of the equation is involved. On the other hand, in the study of second-order transport quantities, such as noise in physical systems, the concept of different "noise sources" is usually introduced, thus tracing back to the fluctuating forces in the Langevin equation.

The formal derivation of Langevin equations from the very microscopic dynamics of a system has been intensively studied using projection-operator techniques.[3-5] These give a good insight in the origin of the different terms of the equations and in the approximations involved in their derivation. They also show the way to generalize these equations including, e.g., memory effects or a coupling of the fluctuating forces.[6-9] The derivation of these Langevin equations needs no further approximations than those already performed in deriving irreversible kinetic equations. The Boltzmann equation for the distribution function of charge carriers can thus be generalized to a Boltzmann-Langevin equation also describing the fluctuations around the stationary state of the distribution function and containing the Boltzmann equation as the equation for the mean values.[10,11] The fluctuating forces are uniquely determined by the same scattering rates entering in the Boltzmann equation. This fact is the reason why the Monte Carlo (MC) technique, originally introduced to solve the Boltzmann equation,[12] can be directly used to study fluctuations without any further assumptions than the knowledge of the scattering rates.[13]

The Boltzmann-Langevin equation is an equation for an infinite set of variables, the occupation number for any state $\mathbf{k}$. In general, however, one is interested only in a very limited set of quantities, for example the lowest moments: density, velocity, and energy of the carriers. The question addressed in this paper therefore is the following: can we find a subspace of "relevant" variables such that the stochastic process in this subspace is still Markovian, or in other words, that the fluctuations in this subspace satisfy a closed set of coupled Langevin equations? For any real semiconductor under far-from-equilibrium conditions, this question cannot be answered from an analytical point of view due to the difficulty in obtaining a solution of the Boltzmann equation, which includes the various scattering processes with their different energy and wave-vector dependencies. On the other hand, the above question can obtain a numerical answer through the MC method which has been shown to be well suited to study the transport in real semiconductors without simplifying assumptions in treating the scattering processes or the strength of the applied fields.

To this purpose we use a MC simulation to calculate first-order and second-order quantities in a nondegenerate semiconductor in which charge transport occurs through a two-level system: the conducting band (here the valence band) and the impurity centers which supply the carriers. From the results, in particular those regarding correlation functions, it emerges that the five variables u (fraction of free carriers), $\mathbf{v}$ (the three components of the velocity), and ε (energy per carrier) to a good approximation indeed form a complete set of relevant variables. We then construct a set of coupled Langevin equations for these variables. Their conceptual simplicity allows us to get a better physical insight into the high-field transport processes, and in particular in the coupling between different variables as well as their corresponding fluctuating forces. This paper complements a previous one,[14] hereafter cited as I, where we have investigated the time dependence of the correlation functions, which is described by the dissipative part of the Langevin equations.

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II. THEORY AND RESULTS

In the following we will restrict ourselves to the case of stationary processes. Let us denote the instantaneous values of the five variables as $P_i(t)$, $i=1,\ldots,5$. We assume that the fluctuations of these variables $\delta P_i(t)=P_i(t)-\langle P_i\rangle$ satisfy the coupled set of linear Langevin equations

$$(d/dt)\delta P_i(t)=-\sum_j \alpha_{ij}\delta P_j(t)+\Gamma_i(t) \qquad (1)$$

with the relaxation matrix α_{ij}, the mean values $\langle P_j\rangle$, and the fluctuating forces $\Gamma_i(t)$. The fluctuating forces, which are taken as δ-correlated in time, have a zero mean value and are characterized by their generalized-diffusion matrix γ_{ij}, that is

$$\langle \Gamma_i(t)\rangle=0\ , \qquad (2a)$$

$$\langle \Gamma_i(t)\Gamma_j(t')\rangle=\gamma_{ij}\delta(t-t')\ . \qquad (2b)$$

Assuming Gaussian fluctuating forces, the Langevin equation (1) is equivalent to the Fokker-Planck equation for the probability distribution $W(\delta P_i,t)$ (Ref. 1),

$$\frac{\partial}{\partial t}W(\delta P_k,t)=\sum_{i,j}\frac{\partial}{\partial\delta P_i}\left[\alpha_{ij}\delta P_j+\tfrac{1}{2}\gamma_{ij}\frac{\partial}{\partial\delta P_j}\right]W(\delta P_k,t)\ . \qquad (3)$$

This explains that indeed γ_{ij} can be interpreted as a generalized-diffusion matrix in the space of the relevant variables.

Given the initial values and initial time derivatives of the set of correlation functions $\Phi_{ij}(t)=\langle\delta P_i(0)\delta P_j(t)\rangle$, the parameters entering in Eqs. (1) and (2) can be calculated according to the following formulas:

$$\alpha_{ij}=D_{ij}/D\ , \qquad (4)$$

$$\gamma_{ij}=\sum_{k,l}(\alpha_{jl}\delta_{ik}+\alpha_{ik}\delta_{jl})\Phi_{kl}(0)\ . \qquad (5)$$

where $d=\det[\Phi_{kl}(0)]$ and D_{ij} is the determinant obtained from D, if in column j the values $\Phi_{kj}(0)$, are replaced by $-(d/dt)\Phi_{ki}(0)$.[15,16] At thermal equilibrium the initial values of the correlation functions $\Phi_{ij}(0)$ can be expressed in terms of the temperature and the chemical potential, thus Eq. (5) represents the generalized Einstein relation.

The MC simulations have been performed for the case of uncompensated p-type Si with an acceptor concentration $N_A=3\times10^{15}$ cm^{-3} at 77 K, where the generation-recombination processes from the shallow impurity levels have been taken into account. Details of the calculations as well as the material parameters used are given in I. The electric field has been varied by more than four orders of magnitude.

Figure 1(a) shows the mean values of the fraction of the free carrier, the longitudinal velocity v_l, and the carrier energy as a function of the electric field. Since we have a cubic semiconductor with an electric field in the $\langle 100\rangle$ direction, the mean value of the transverse velocity v_t remains always zero. The fraction of free carriers increases with increasing field due to the suppression of recombination processes which occur practically only from the bottom of the band. At high fields it reaches unity. The longitudinal average velocity, after an initial Ohmic increase, tends to saturate at fields above some 10^4 V/cm. The mean energy shows, at intermediate fields, only a slight increase and at high fields, when the cooling due to optical phonons becomes less efficient, increases strongly.

From these mean values the phenomenological lifetime τ_u, momentum relaxation time τ_{vl}, and energy relaxation time τ_ε can be obtained by using the results obtained from the balance equations[17]

$$\tau_u=\langle u\rangle\tau_g\ , \qquad (6a)$$

$$\tau_v=m\langle v_l\rangle/eE\ , \qquad (6b)$$

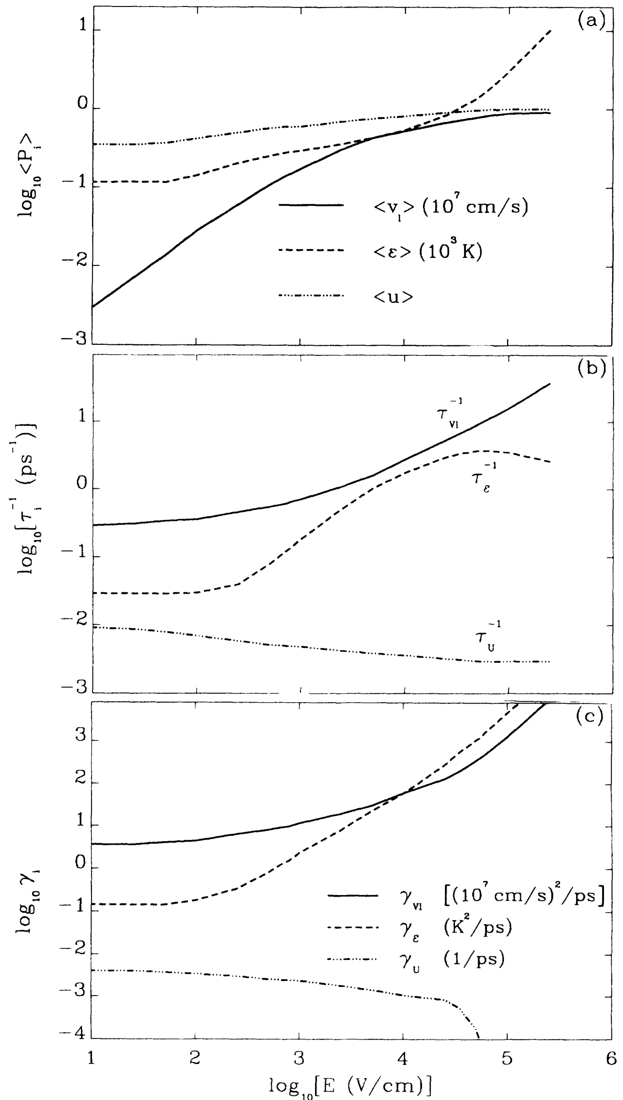

FIG. 1. (a) Mean values of the relevant variables, (b) phenomenological relaxation rates, and (c) phenomenological generalized diffusivities as a function of the electric field applied parallel to the $\langle 100\rangle$ crystallographic direction. Values are obtained from a Monte Carlo simulation for the case of p-type Si at 77 K with an acceptor concentration of $N_A=3\times10^{15}$ cm^{-3}.

$$\tau_\varepsilon = (\langle \varepsilon \rangle - \tfrac{3}{2} k_B T)/e \langle v_l \rangle E \ . \tag{6c}$$

Here τ_g is the mean generation time, m is the carrier effective mass, and T the lattice temperature. The inverse of these relaxation times is plotted in Fig. 1(b). We note the nonmonotonic behavior of the energy relaxation rate which exhibits a maximum at about 5×10^4 V/cm.

In order to describe the variance of the distribution of the relevant variables, we can define the effective diffusivities for the respective variables as

$$\gamma_u = 2 \langle \delta u^2 \rangle / \tau_u \ , \tag{7a}$$

$$\gamma_{vl} = 2 \langle \delta v_l^2 \rangle / \tau_v \ , \tag{7b}$$

$$\gamma_\varepsilon = 2 \langle \delta \varepsilon^2 \rangle / \tau_\varepsilon \ . \tag{7c}$$

These are shown in Fig. 1(c). In the definitions given above, it is assumed that the fluctuations and relaxations of the variables are independent. Their field dependence will serve as a reference when discussing the full relaxation and diffusion matrices in the following.

Figure 2 shows the field dependence of the relaxation matrix, as calculated from the correlation functions. The diagonal components are plotted in Fig 2(a). In the absence of coupling they would represent the respective relaxation rates for the fraction of free carriers, their velocities and energy. Indeed, their field dependence is qualitatively in agreement with the phenomenological rates in Fig. 1(b). Their field dependence reflects the presence of hot-electron conditions. At increasing fields α_{uu} tends to decrease because of the field-assisted ionization mechanism. The velocity relaxation rates tend to increase because of the increased efficiency of the scattering mechanisms. The energy relaxation rate exhibits a maximum and then decreases at the highest field because of the smaller efficiency of scattering to dissipate the excess energy gained by the field.

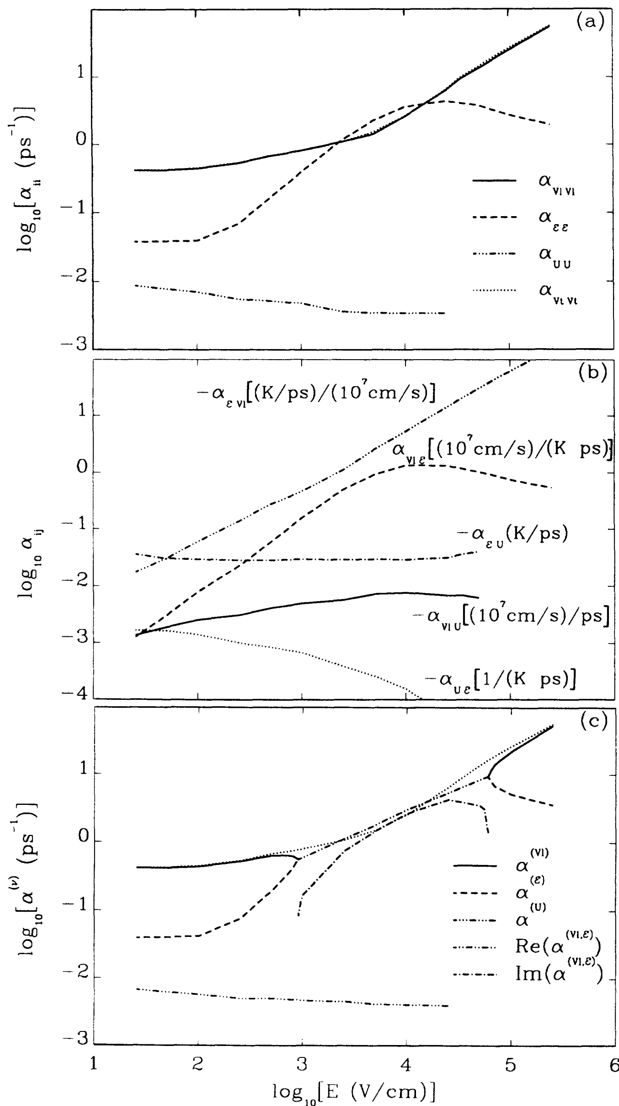

FIG. 2. Relaxation matrix coefficients as a function of the electric field. (a) Diagonal components, (b) off-diagonal components, and (c) eigenvalues.

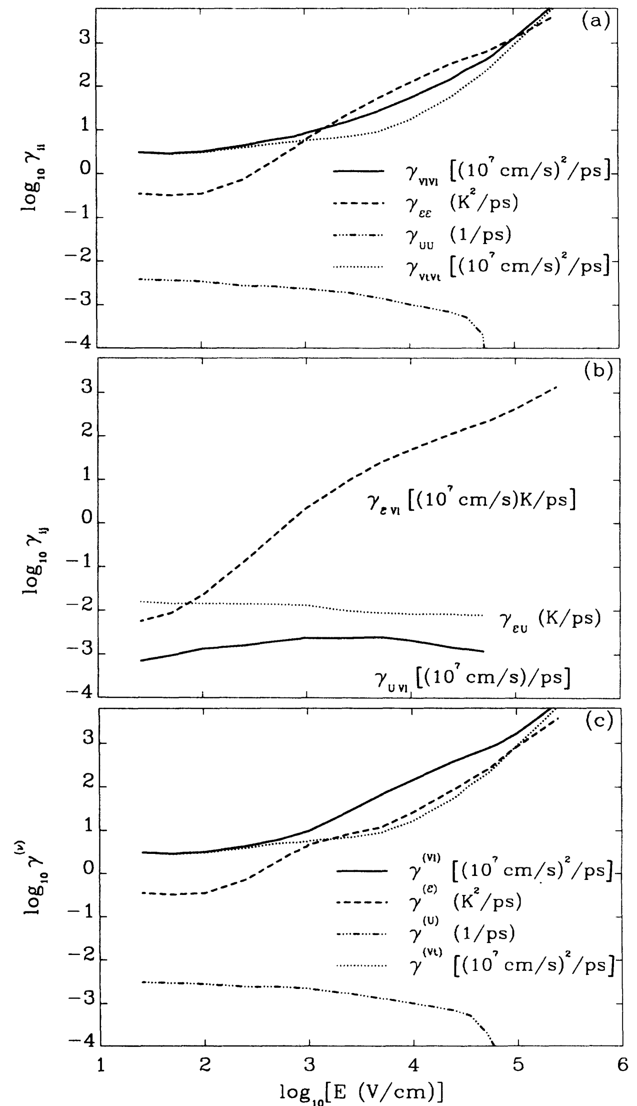

FIG. 3. Generalized-diffusion matrix coefficients as a function of the electric field. (a) Diagonal components, (b) off-diagonal components, and (c) eigenvalues.

The off-diagonal components, plotted in Fig. 2(b), describe the coupling between the relaxation of these variables. At vanishing fields only the coupling between the carrier number and their energy remains, while for symmetry reasons all couplings with a velocity component vanish. The coupling between energy and longitudinal velocity turns out to be the most important since it increases systematically with field. The coupling between u and v_l is not reported because its magnitude is so small that it cannot be detected with sufficient accuracy.

In order to interpret the coupling in the relaxation processes, we have calculated the eigenvalues of the matrix α as a function of the electric field. They determine the relevant time scales for the dynamics. Since this matrix is not symmetric, the eigenvalues need not be real, but there can be also a pair of conjugate complex values. Indeed, it turns out that this occurs at intermediate field strengths. These complex values can be attributed to a streaming character of the transport and has been discussed in detail in I. In any case, we remark that at the lowest and highest fields the eigenvalues well agree with both the phenomenological rates as well as with the diagonal components of the relaxation matrix.

Figure 3 show the field dependence of the diffusion matrix as calculated from the correlation functions. The diagonal components are plotted in Fig. 3(a). Here γ_{uu} is decreasing with increasing field and approaches zero when the fraction of free carriers approaches unity, since in this limit the corresponding fluctuations vanish. The other diagonal components are increasing with increasing field showing the increasing efficiency of the corresponding fluctuating forces with increasing carrier energy. Again, in the absence of coupling, they would agree with the phenomenological diffusivities shown in Fig. 1(c).

Figure 3(b) shows the off-diagonal components; since the diffusion matrix is always symmetric there are only three independent components. As in the case of the relaxation matrix, at vanishing fields only the correlation in fluctuations between energy and carrier number remains finite, the other components tending to zero linearly with the field. At increasing fields, the correlation between velocity and energy fluctuating forces is strongly increasing while the other two components remain practically constant with field. Thus, the former one plays the most important role.

In Fig. 3(c) we report the eigenvalues of the diffusion matrix. They determine the strength of the independent fluctuating forces in the space of the relevant variables, and are always real due to the symmetric character of γ_{ij}. The corresponding eigenvectors give the linear combination of the variables on which these uncorrelated forces act.

III. CONCLUSIONS

This paper has presented a detailed analysis of hot-carrier transport and fluctuations in a doped semiconductor in terms of a Langevin equation approach. Using a Monte Carlo simulation, first and second-order transport quantities have been calculated. From these results a set of coupled linear Langevin equations has been constructed. This method has enabled us to obtain the relaxation matrix associated with dissipation properties as well as the generalized-diffusion matrix associated with fluctuating forces. Calculations have been applied to the case of p-type Si at 77 K in the presence of generation-recombination processes from shallow traps. A detailed comparison between phenomenological values and those obtained from the present rigorous approach has been carried out.

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