# NUMERICAL SOLUTION OF THE PERTURBED BOLTZMANN EQUATION IN FREQUENCY AND TIME DOMAINS

J. C. Vaissiere, J. P. Nougier, L. Varani, P. Houlet
*Centre d'Electronique de Montpellier,*
*Université Montpellier II, 34095 Montpellier Cedex 5, France*

L. Hlou
*Faculté des Sciences de Kénitra,*
*Kénitra, Morocco*

L. Reggiani
*Dipartimento di Fisica, Università di Modena,*
*Via Campi 213/A, 41100 Modena, Italy*

E. Starikov, P. Shiktorov
*Semiconductor Physics Institute,*
*Goshtauto 11, 2600 Vilnius, Lithuania*

**Abstract**

We present two original methods which yield the small-signal response around the d.c. bias in bulk semiconductors, using direct numerical resolutions of the perturbed Boltzmann equation. The first method operates in the frequency domain. An a.c. sinusoidal electric field perturbation superimposed to the d.c. field produces an a.c. perturbation of the distribution function which is computed at each frequency. The second method operates in the time domain. A step electric field perturbation is superimposed at time t=0 to the d.c. field. The resulting perturbations of the distribution function and of the average velocity are then computed as a function of time. These methods are applied to the case of holes in silicon at T=300 K under hot-carrier conditions and used to compute the differential-mobility spectrum.

## I. INTRODUCTION

Small-signal response functions around the bias point are known to play a fundamental role in the investigation of hot-carrier transport and noise in bulk semiconductors. In the time domain they reflect both dynamic and relaxation processes inherent to the hot-carrier system and can be used for the detailed investigation of kinetic phenomena. In the frequency domain they provide the differential mobility spectrum which is necessary for several purposes, such as: to evaluate a possibility of amplification and generation, to calculate the gain or the absorption coefficients, to obtain the noise temperature using additionally the spectral density of velocity fluctuations, etc. To date the most comprehensive theoretical analysis of these phenomena is based on numerical solutions of the Boltzmann Equation (BE), typically by means of Monte Carlo simulations. However, together with evident advantages, the Monte Carlo method has also inherent shortcomings mainly related to the stochastic nature of the procedure: as a matter of fact, the standard Monte Carlo scheme meets difficulties in calculating with high accuracy quantities on a hydrodynamic time scale such as the small-signal kinetic coefficients. Other alternative methods deals with the steady state hot-carrier transport and often cannot be reformulated in terms of the time-dependent BE. In this communication, we present two original deterministic (as opposite to stochastic) methods which yield the small-signal response around the d.c. bias in bulk semiconductors, using direct numerical resolutions of the perturbed BE.

## II. THEORY

The distribution function $f(\mathbf{k},t)$ of carriers in homogeneous nondegenerate semiconductors with a uniform external applied electric field $\mathbf{E}(t)$ is the solution of the time-dependent BE. In a constant electric field $\mathbf{E}_s$ of magnitude $E_s$, $f(\mathbf{k},t)$ takes the stationary value $f_s(\mathbf{k})$. If a small electric field $\delta\mathbf{E}(t)$ is superimposed on $\mathbf{E}_s$, it produces a variation of the distribution function $\delta f(\mathbf{k},t)$ which is the solution of the perturbed BE in time domain [1]:

$$\frac{\partial}{\partial t}\delta f(\mathbf{k},t) + \frac{e\mathbf{E}_s}{\hbar}\cdot\nabla_k\delta f(\mathbf{k},t) - C\delta f(\mathbf{k},t) = -\frac{e\delta\mathbf{E}(t)}{\hbar}\cdot\nabla_k f_s(\mathbf{k}) \tag{1}$$

where $\hbar$ is the reduced Planck constant and $C$ the collision operator.

### 1. Harmonic-Response Method

When the perturbation is sinusoidal [$\delta \mathbf{E}_{har} = \delta \mathbf{E} exp(i\omega t)$], the response is also sinusoidal [$\delta f(\mathbf{k},t) = \delta f(\mathbf{k},\omega) exp(i\omega t)$]. Then from Eq. (1) we obtain the perturbed BE in frequency domain [1]:

$$i\omega \delta f(\mathbf{k},\omega) + \frac{e\mathbf{E}_s}{\hbar} \cdot \nabla_k \delta f(\mathbf{k},\omega) - C\delta f(\mathbf{k},\omega) = -\frac{e\delta \mathbf{E}}{\hbar} \cdot \nabla_k f_s(\mathbf{k}) \tag{2}$$

From the knowledge of $\delta f(\mathbf{k},\omega)$ we obtain the Fourier transform $\delta \mathbf{v}(\omega)$ of $\delta \mathbf{v}(t)$ as:

$$\delta \mathbf{v}(\omega) = \left[ \int \mathbf{v}(\mathbf{k}) \delta f(\mathbf{k},\omega) d^3k \right] \left[ \int f_s(\mathbf{k}) d^3k \right]^{-1} \tag{3}$$

The complex quantities $\delta \mathbf{v}(\omega)$ and $\delta \mathbf{E}$ are linearly related through the a.c. differential mobility $\mu(\omega)$ as: $\delta \mathbf{v}(\omega) = \mu(\omega) \delta \mathbf{E}$.

By assuming a spherical symmetry of the band model the perturbation term $\delta f(\mathbf{k},\omega)$ can be written as $\delta f(k,\theta,\omega)$ where $k = |\mathbf{k}|$ and $\theta = (\mathbf{E},\mathbf{k})$. After discretization, the gradient and the collision operators in Eq. (2) appear as linear combinations of $\delta f(k,\theta,\omega)$. In practice, the computed quantity is $\delta f_E = \delta f(k,\theta,\omega)/\delta E$, represented by a column matrix $[\delta f_E]$ which has a real part $[\delta f_E]_{re}$ and an imaginary part $[\delta f_E]_{im}$ calculated as:

$$\begin{aligned} [\delta f_E]_{re} &= [A] \left( [A]^2 + \omega^2 [I] \right)^{-1} [g] \\ [\delta f_E]_{im} &= -\omega \left( [A]^2 + \omega^2 [I] \right)^{-1} [g] \end{aligned} \tag{4}$$

where the square matrix $[A]$ represents the discretized operator $[(e\mathbf{E}_s/\hbar)\nabla_k - C]$, the column matrix $[g]$ represents the discretized vector $(e/\hbar)\nabla_k f_s(\mathbf{k})$, and $[I]$ is the identity matrix. The unknowns on the left-hand side of Eq. (4) are easily obtained using standard numerical techniques (Gauss procedure). This method enables to use an arbitrary value of $\delta E$: indeed, since the computed quantity is $\delta f_E$ the actual value of $\delta E$ does not appear in Eq. (4). Furthermore, the solution of Eq. (4) requires a specific program. We remark also that the solution of Eq. (2) presents difficulties for low frequencies ($< 10^8\ Hz$) because its associated determinant becomes small [2].

### 2. Impulse-Response Method

In this case we apply a step-like electric field perturbation, $\delta \mathbf{E}_{step}(t) = \delta \mathbf{E} u(t)$ where $u(t)$ is the step function $u(t) = 1$ if $t \geq 0$ and $u(t) = 0$ if $t < 0$. The step distribution response $\delta f_{step}(\mathbf{k},t)$ is then the solution of Eq. (1), and the step velocity response $\delta \mathbf{v}_{step}(t)$ is given by Eq. (3) where $\delta f(\mathbf{k},\omega)$ is replaced by $\delta f_{step}(\mathbf{k},t)$. To obtain the transient distribution function $\delta f_{step}(\mathbf{k},t)$, we first solve (using a direct method [3]) the transient BE in the constant field $E_s$, so calculating $f_s(\mathbf{k})$. Then we solve the transient BE in a constant field $E_s + \delta E$, with the initial distribution equal to $f_s(\mathbf{k})$, thus evaluating the transient $f(\mathbf{k},t)$. The step distribution response is then calculated by difference as $\delta f_{step}(\mathbf{k},t) = f(\mathbf{k},t) - f_s(\mathbf{k})$. Then $\delta \mathbf{v}(\omega)$ is calculated as:

$$\delta \mathbf{v}(\omega) = \int_{-\infty}^{+\infty} \frac{d\delta \mathbf{v}_{step}(t)}{dt} exp(-i\omega t) dt \tag{5}$$

Thus Eq. (5) provides a second method to obtain the a.c. differential mobility.

This method can be used by employing the same program developed for the direct solution of the BE [3] or the Scattered Packet Method [4] since the accuracy of these methods is sufficient to compute precisely $d\delta \mathbf{v}_{step}(t)/dt$. On the other hand, with respect to the harmonic-response method, it is necessary to take a value of $\delta E$ large enough (typically between 1 and 10 % of $E_s$). This calculation can take advantage of an acceleration technique described in Ref. [5].

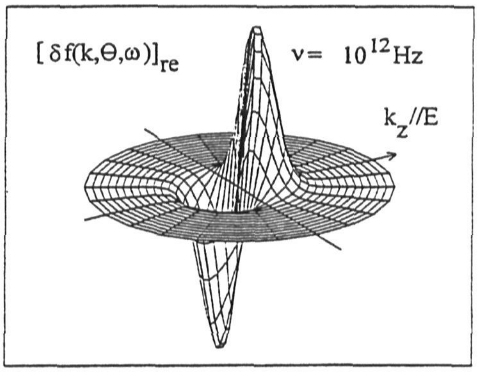


Fig. 1 - *3-D representation of the real part of the perturbation of the distribution function $[\delta f(k,\theta,\omega)]_{re}$ (harmonic-response method), in arbitrary scales, at frequency $\nu = \omega/2\pi = 10^{12}$ $Hz$, for holes in Si, $T = 300$ $K$, $E_s = 10$ $kV/cm$, corresponding to a perturbing field $\delta E = 1$ $V/cm$.*

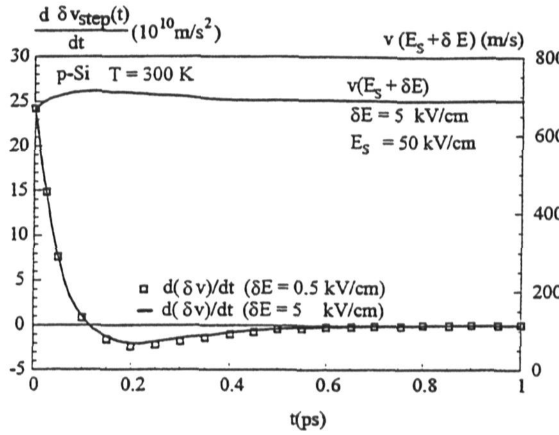


Fig. 2 - *Drift velocity (right scale) and time derivative of the transient response of the drift velocity (left scale). Calculations refer to holes in Si with $T = 300$ $K$, $E_s = 50$ $kV/cm$ and the reported values of $\delta E$.*

## III. RESULTS

The above procedures are used to calculate the small-signal response characteristics of holes in Si at T=300 K. The microscopic model is based on a single spherical nonparabolic-band and considers scattering with acoustic and non-polar optical phonon mechanisms as described in Ref. [6].

Figure 1 shows the real part of the perturbation of the distribution function $\delta f(k,\theta,\omega)$ calculated using the harmonic-response method [see Eq. (4)]. Each radial curve gives the variation of $\delta f(k,\theta,\omega)$ at a given value of the angle $\theta$. In analogy with the Drude model for the a.c. conductivity, the real part describes the dissipative contribution which is in phase with the field while the imaginary part (here not reported) describes the optical contribution which is in quadrature with the field. Figure 2 reports the time dependence of the drift velocity when at time $t = 0$ a step electric field is superimposed to $E_s$. The same figure shows the time derivative of the transient response of the drift velocity for two different values of $\delta E$ (we notice that, in order to compare the two curves, the reported values have been divided by $\delta E/(1\ V/m)$). The excellent agreement observed shows that a $\delta E$ of few percents of $E_s$ can be employed in order to compute the linear response of the system. Figure 3 shows the time-derivative of the velocity response-function $\delta \mathbf{v}_{step}(t)$ (divided by $\delta E/(1\ V/m)$) whose Fourier transform gives $\delta \mathbf{v}(\omega)$ according to Eq. (5). At time t=0, all curves have practically the same value of $[d\delta \mathbf{v}_{step}(t)/dt]_{t=0} = e\delta E/m^*$, where $m^*$ is the effective mass. The small changes at $t = 0$ are due to the non-parabolicity of the band. At zero and low electric fields, the shape of the velocity response- function is practically exponential with a characteristic time constant which corresponds to momentum relaxation. At higher fields the shape becomes more complicated by exhibiting a negative part which is understood as follows. At the initial stage of the velocity relaxation, carriers obtain extra velocity, since their initial momentum relaxation time $\tau_p$ is somewhat longer than that in the new steady-state. Then, the energy relaxation affects $\tau_p$ (i.e. $\tau_p$ becomes shorter) and this extra velocity is lost. Therefore, the energy relaxation is responsible for the negative contribution of the velocity response-function.

The harmonic and impulse response methods are further used to calculate the differential mobility spectrum which is reported in Fig. 4. The circles and the solid line show the a.c. mobility computed respectively with the harmonic- and the impulse-response method. The agreement between the two techniques is excellent, thus validating the present approach. In particular, from Fig. 4 significant deviations from the simple Drude slope of $\mu_r$ and $\mu_i$ are evidenced. This peculiarity is explained as follows. At zero and low d.c. electric fields the impulse velocity response decreases monotonously with increasing time (see Fig. 3), and the characteristic relaxation time involved is

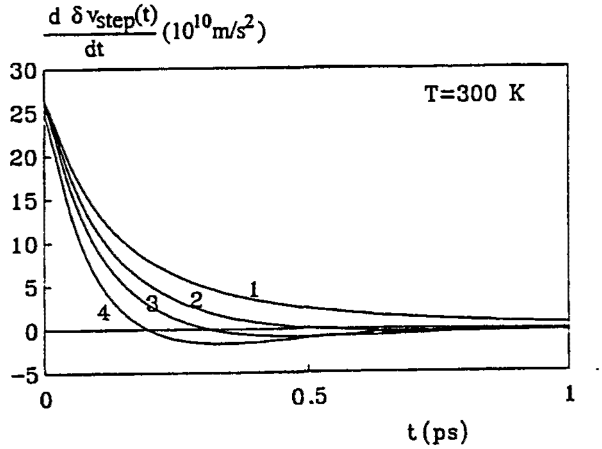


Fig. 3 - *Time derivative (divided by $\delta E/(1\ V/m)$) of the transient response of the drift velocity. Calculations refer to holes in Si with $T$ = 300 $K$, and $\delta E$ = 1 $V/cm$ for $E_s$ = 0, and $\delta E = 0.1E_s$ otherwise. 1: $E_s = 0$; 2: $E_s$ = 5 $kV/cm$; 3: $E_s$ = 10 $kV/cm$; 4: $E_s$ = 20 $kV/cm$.*

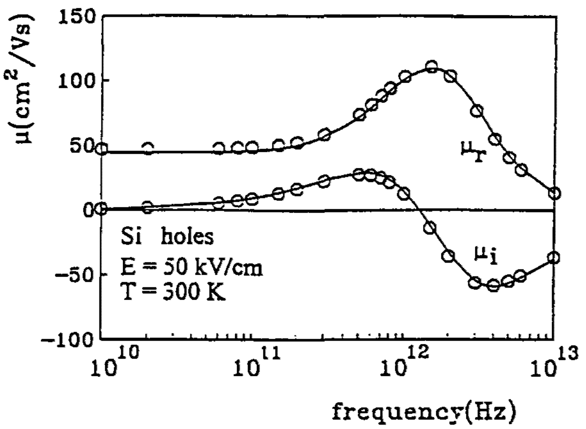


Fig. 4 - *Real part $\mu_r$ and imaginary part $\mu_i$ of the a.c. mobility for holes in Si at an applied d.c. electric field $E_s$ = 50 $kV/cm$. Circles : harmonic-response method with $\delta E$ = 1$V/cm$; Solid line: impulse response-method with $\delta E$ = $0.1E_s$.*

then the momentum relaxation time. At higher fields, the energy relaxation time begins to play a role. This results in a negative value of $[d\delta v_{step}(t)/dt]$, which corresponds to a bump in $\mu_r$ With increasing electric field, $\mu_r$ increases in the low frequency region, which implies a positive value of $\mu_i$ then decrease resulting in a negative value of $\mu_i$.

## IV. CONCLUSIONS

We have presented two methods for calculating the small-signal response around the d.c. bias in bulk semiconductors, using direct numerical resolutions of the perturbed Boltzmann equation. Both methods have been validated for the case of holes in Silicon and proven to give exactly the same results when used to compute the differential mobility spectrum. The harmonic-response method requires to perform a simulation for each frequency of interest while the impulse-response method gives directly the whole spectrum within one simulation. The methods are deterministic and therefore overcome the difficulties of the stochastic methods (such as Monte Carlo simulations) in calculating with high accuracy transport parameters on a hydrodynamic time scale.


## ACKNOWLEDGMENTS

This work has been performed within the *European Laboratory for Electronic Noise* (ELEN) and supported by the Commission of European Community through the contracts ERBCHRXCT920047 and ERBCHBICT920162. Partial support from the italian *Consiglio Nazionale delle Ricerche* (CNR) and the *Centre de Competences en Calcul Numériques Intensif* (C3NI) is gratefully acknowledged.


## REFERENCES


[1] J. C. Vaissiere, J. P. Nougier, L. Varani, P. Houlet, L. Hlou, E. Starikov, P. Shiktorov and L. Reggiani, Phys. Rev., in press.

[2] J. P. Aubert, J.C. Vaissiere and J.P. Nougier, J. Appl. Phys. **56**, 1128 (1984).

[3] P.A. Lebwohl, P.M. Marcus, Solid State Commun. **9**, 1671 (1971).

[4] J.P. Nougier, L. Hlou, P. Houlet, J.C. Vaissiere and L. Varani, Proceedings of the 3$^{rd}$ *Int. Workshop on Computational Electronics*, Portland (1994).

[5] L. Hlou, Thèse de Doctorat, Universitè Montpellier II (France), 1993 (available upon request).

[6] J. C. Vaissiere, Thèse de Doctorat ès Sciences, Universitè Montpellier II (France), 1986 (available upon request).