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Possible Generation of Transient THz Electronic Drift Effects in a Semiconductor by a High Electric Field

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Abstract. — Using the Boltzmann equation formalism for a simple semiconductor model, the transient drift velocity of the electrons is computed when a high uniform electric field is suddenly turned on. Rapid oscillations superimposed on an overshoot behaviour are obtained. It is showed that this behaviour results from the combined action of the field and of the electron-phonon interaction.

Résumé. — En utilisant le formalisme de l’équation de Boltzmann pour un modèle simple de semiconducteur, on a calculé la vitesse de “drift” transitoire des électrons quand le système est soumis à l’action brusque d’un champ électrique fort et uniforme. On a obtenu des oscillations rapides superposées à une évolution du type “overshoot” et on a démontré qu’elles résultent de l’action combinée du champ extérieur et des interactions électron-phonon.

1. Introduction

It has recently become possible to fabricate small size electronic devices. The short distances involved lead to high electric fields and the electronic transport takes place over very short time scales. Consequently, the study of the transient effects became crucial for the understanding of the operation of such devices and in the effort to increase their speed.

The first steps were mainly theoretical, based both on Monte Carlo simulations and solutions of the Boltzmann transport equations [1]. Some of these investigations [2, 3] predicted velocity overshoot phenomena as an important transient effect to be used in faster devices.

Recently, optical techniques have been developed in order to achieve the appropriate spatial and temporal resolutions for the experimental study of the problem [4–7]. These methods opened the way to direct investigation of the transient behaviour which now seems to be more complicated than that theoretically predicted [5, 6].

In the present paper, a simple theoretical method (based on the Boltzmann equation) will be used in order to explain the overshoot of the drift velocity. We will also prove the possible

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existence of an oscillatory shape of the peak in the THz domain, which is influenced by the types of scattering mechanisms of the electrons.

In practice this oscillatory behaviour may lead to electromagnetic pulses (which in fact, have already been used in some investigations of the transient phenomena [6]), and which could contain useful information about the electronic interactions.

2. The Transport Equation

Let us suppose that a sample of n-type nondegenerate semiconductor is subject to an external uniform electric field. The general form of the transport equation for electrons will be:

$$ \frac{\partial f}{\partial t} = \hat{F} f - \hat{C} f, $$

where

$$ \hat{F} f = \frac{|e| E}{\hbar} \frac{\partial f}{\partial k} $$

is the field operator describing the action of the applied electric field $E$. $\hat{C}$ is the general collision operator for the electrons (which for nondegenerate semiconductors can be considered as linear and homogeneous), and $f(k, t)$ is the position independent electronic distribution function for which the normalisation condition

$$ \frac{V_0}{4\pi^3} \int f(k, t) dk = 1, \quad (\forall t) $$

must hold [8]. The integral is taken over the Brillouin zone and $V_0$ is the volume of the primitive cell of the lattice.

In order to simplify the discussion we shall consider $E$ as suddenly applied at $t = 0$ and constant thereafter. The initial form of the distribution function will then be the equilibrium form, which, for nondegenerate semiconductors, is well approximated by [8]:

$$ f_0(k) = \frac{1}{2V_0} \left( \frac{a^2 \beta}{\pi} \right)^{3/2} \exp \left( -\frac{a^2}{4\pi^2 \beta k^2} \right) $$

where $a$ is the constant of the (cubic) lattice and

$$ \beta = \frac{2\pi^2 \hbar^2}{a^2 m k_B T} $$

Here $m$ is the effective mass of the electrons and $k_B$ is the Boltzmann constant.

Since the Brillouin zone has an inversion symmetry around its centre, the function $f(k, t)$ can always be written as a sum of its symmetric and antisymmetric parts [9]:

$$ f_+(k, t) = \frac{1}{2} [f(k, t) + f(-k, t)] $$

$$ f_-(k, t) = \frac{1}{2} [f(k, t) - f(-k, t)]. $$

The drift velocity defined by [10]:

$$ \mathbf{v}_d(t) = \frac{V_0}{4\pi^3} \int \mathbf{v}(k) f(k, t) dk $$
should then be produced only by \( f_- (k, t) \) since the group velocity of the electrons is given by [10]:

\[
v(k) = \frac{1}{\hbar} \frac{\partial}{\partial k} \varepsilon(k),
\]

and since the electronic energy band can be considered as isotropic:

\[
\varepsilon(k) = \varepsilon(k).
\]

One then obtains:

\[
v_d(t) = \frac{V_0}{4\pi^2\hbar} \int \frac{\partial \varepsilon(k)}{\partial k} f_-(k,t)\,dk
\]

which implies that an equation for \( f_-(k, t) \) is needed in order to calculate the drift.

Writing (1) for \( k \) and for \((-k)\), adding and subtracting the obtained equations, one arrives at the following equivalent system:

\[
\frac{\partial f_-}{\partial t} = \hat{F} f_+ - \hat{C} f_-
\]

\[
\frac{\partial f_+}{\partial t} = \hat{F} f_- - \hat{C} f_+
\]

In obtaining this, one must use the fact that the action of \( \hat{F} \) or \( \hat{C} \) on a function reverses and respectively preserves its symmetry. This is obvious for \( \hat{F} \) from the definition (2) and for \( \hat{C} \) it can be demonstrated for every scattering mechanism of interest in nondegenerate semiconductors [11].

Since the field is constant and since \( k \) and \( t \) are independent variables [12], the time derivative commutes with \( \hat{F} \) and \( \hat{C} \) operators, and thus the following equation can be obtained from (12) and (13):

\[
\frac{\partial^2 f_-}{\partial t^2} = \hat{F}^2 f_- - \hat{C} \frac{\partial f_-}{\partial t} - \hat{F} \hat{C} f_+
\]

As it will become clear from the more detailed analysis in the next section, the contribution of the last term in (14) is very small. For example, if the interaction is elastic, it vanishes.

Therefore, neglecting this term in (14), the remaining contains only \( f_- \), and its form is close to an equation for a damped wave propagating in the reciprocal space in the field direction. This is clearer if one uses in (14) the projection \( k_\parallel \) of \( k \) in this direction:

\[
\frac{\partial^2 f_-}{\partial t^2} = \left( \frac{e}{\hbar} E \right)^2 \frac{\partial^2 f_-}{\partial k_\parallel^2} - \hat{C} \frac{\partial f_-}{\partial t}
\]

If the applied electric field is strong enough and if some suitable boundary and initial conditions are satisfied by \( f_- \), then an oscillatory solution is possible for (15), leading to a similar behaviour for the transient drift velocity (11).

The boundary condition may be derived from (3) if one takes into account the relation

\[
\int \hat{C} f(k, t)\,dk = 0, \quad (\forall \, t),
\]

which expresses the fact that the \( \hat{C} \) operator can only redistribute the conduction electrons among their bounded set of states. This statement can be verified directly on the general form of \( \hat{C} \) [11].
By integrating both members of (1) over the Brillouin zone, and by taking advantage of (3) and (16), and using the Gauss Theorem, one finds that

$$\int_{\Sigma} f(k,t)(\mathbf{E} \cdot d\Sigma) = 0, \quad (\forall t),$$

(17)

where $\Sigma$ is the boundary of the Brillouin zone and $d\Sigma$ is its outward oriented surface element. Since the integral for $f_+(k,t)$ vanishes on the symmetric boundary $\Sigma$, it follows from (17) that

$$\int_{\Sigma} f_-(k,t)(\mathbf{E} \cdot d\Sigma) = 0, \quad (\forall t),$$

(18)

which represents the boundary condition for the function $f_-$.

As for the initial conditions one may use the original form (4) of the distribution and obtain

$$f_-(k,t=0) = 0.$$  

(19)

Then, from (12) it follows that

$$\frac{\partial f_-}{\partial t}(k,t=0) = \hat{F} f_0(k).$$  

(20)

3. The Solution of the Equation (14) and the Drift Velocity of the Electrons

In order to obtain numerical results, one must use certain approximations. First, we shall suppose a simple parabolic band structure for the electrons:

$$E(k) = \frac{\hbar^2}{2m} k^2.$$  

(21)

This will avoid unnecessary complications.

We then notice the axial symmetry of our problem around the field direction and use a Legendre polynomials expansion for the $\cos \theta$ dependence of $f(k,t)$ ($\theta$ being the angle between $k$ and $\mathbf{E}$). From this we shall retain only the first two terms, which is a frequently adopted approximation [10,11,13]:

$$f(k,t) \approx \varphi_0(k,t) + \varphi_1(k,t) \cos \theta$$

(22)

It follows by (6) and (7), that

$$f_+(k,t) \approx \varphi_0(k,t)$$

(23)

and

$$f_-(k,t) \approx \varphi_1(k,t) \cos \theta$$

(24)

As for the collision operator $\hat{C}$, we shall consider the electron-acoustical phonon and electron-polar optical phonon to be the dominant interactions and write $\hat{C}$ as a sum of $\hat{C}_{ac}$ and $\hat{C}_{po}$ [10,11,13]:

$$\hat{C}_{ac} = \frac{|e| \alpha^2}{4\pi^2} E_{ac} k \left[ f(k,t) - \frac{1}{4\pi} \int_0^{2\pi} \sin \theta' d\theta' \int_0^{2\pi} f(k,\theta',\varphi',t) d\varphi' \right]$$

(25)

$$\hat{C}_{po} = \frac{|e|}{4\pi \hbar} E_{po} \int dk' \left[ n_0 f(k,t) - (1+n_0) f(k',t) \frac{\delta \left( k' - \sqrt{k^2 + k_0^2} \right)}{|k' - k|^2} \sqrt{k^2 + k_0^2} 
+ \Theta(k - k_0) \frac{(1+n_0) f(k,t) - n_0 f(k',t) \delta \left( k' - \sqrt{k^2 - k_0^2} \right)}{|k' - k|^2} \sqrt{k^2 - k_0^2} \right]$$

(26)
The symbols are defined as follows:

\[ \Theta(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0, \end{cases} \]

\[ n_0 = \left( \exp \left( \frac{\hbar \omega_0}{k_B T} \right) - 1 \right)^{-1}, \]

\[ k_0 = \frac{2\pi}{a} \sqrt{\frac{2m\omega_0}{\hbar}}, \]

\[ E_{ac} = \frac{4\pi \varepsilon_1^2 k_B T}{|e|a^2 \hbar^2 \rho s^2}, \]

\[ E_{po} = \frac{|e|m\omega_0}{\hbar} (\varepsilon_1 - \varepsilon_\infty), \]

where \( \varepsilon_1 \) is the deformation potential constant, \( \rho \) is the crystal density, \( v_s \) and \( \omega_0 \) are the mean sound velocity and the mean optical phonons angular frequency, and \( \varepsilon_\infty, \varepsilon_s \) are the high frequency and static dielectric permitivities. In (25) and (26) the nondegeneracy of the electronic system was used. Furthermore, in (25) the electron - acoustical phonon interaction was considered as elastic.

Using (23) and (24) in (25) one can conclude that

\[ \hat{C}_{ac} f_+ = 0 \]

\[ \hat{C}_{ac} f_- = \frac{|e|a^2}{4\pi^2 \hbar^2} E_{ac} k \varphi_1(k,t) \cos \theta \]

In order to obtain, in a simple form, the action of \( \hat{C}_{po} \) on \( f_{\pm} \), the functions were expanded in power series of \( k/k_0 \) for \( k < k_0 \), and of \( k_0/k \) for \( k > k_0 \), and only the terms up to the first order were retained:

\[ \hat{C}_{po} f_+ \approx \frac{2|e|}{\hbar} E_{po} \frac{1}{k_0} \left[ n_0 \varphi_0(k,t) - (1 + n_0) \varphi_0(k_0,t) \right] \Theta(k_0 - k) \]

\[ \hat{C}_{po} f_- \approx \frac{2|e|}{\hbar} E_{po} \left[ \frac{n_0}{k_0} \Theta(k_0 - k) + \frac{n_0 + 1/2}{k_0} \Theta(k - k_0) \right] \varphi_1(k,t) \cos \theta \]

Using (24), (32-35) in the equation (14), and making the substitution,

\[ \varphi(k,t) = \sqrt{k} \varphi_1(k,t), \]

we obtain

\[ \ddot{\varphi} + 2\dot{\varphi} E_c(k) - \frac{3}{2} \left( \frac{\hbar E}{k} \right) \frac{1}{k} \left[ (k \varphi')' - \frac{9}{4} \frac{\varphi'}{k} \right] + \varphi A_c(k) = 0, \]

where

\[ E_c(k) = \frac{|e|}{2\hbar} \left[ \left( \frac{a}{2\pi} \right)^2 E_{ac} k + 2E_{po} \left( \frac{2n_0}{k_0} \Theta(k_0 - k) + \frac{n_0 + 1/2}{k} \Theta(k - k_0) \right) \right], \]

\[ A_c(k) = \left( \frac{e^2}{\hbar} \right) \frac{2n_0}{k_0} E_{po} \left[ \left( \frac{a}{2\pi} \right)^2 E_{ac} k + \frac{2n_0}{k_0} E_{po} \right] \Theta(k_0 - k), \]

and by \( \dot{\varphi} \) and \( \varphi' \) we mean the time and \( k \) derivatives respectively. The last term in (37) originates from the term \( \hat{F} \hat{C} f_+ \) of (14) where \( \varphi_0' \) was substituted from (12), if we use (23) and (24).
The boundary and the initial conditions for $\varphi$ can be deduced from (18), (19) and (20). Substitution of (24) in (18), assuming that the Brillouin zone can be approximated by a sphere of radius $2\pi/a$, gives

$$\varphi\left(\frac{2\pi}{a}, t\right) = 0, \quad (\forall t).$$

We also have from (36) that

$$\varphi(0, t) = 0, \quad (\forall t),$$

if we notice that $\varphi_1$ is finite at $k = 0$ (in fact it vanishes by (7) and (24)).

Then by (19), (24) and (36) one can deduce

$$\varphi(k, t = 0) = 0,$$

and by (20), (24) and (36) it follows that

$$\varphi(k, t = 0) = \frac{|e|E}{h} \sqrt{k} \frac{\partial f_0(k)}{\partial k}$$

The structure of the equation (37) and the boundary conditions (40) and (41) suggest a solution expanded in a series of Bessel functions of $3/2$ index [14]:

$$\varphi(k, t) = \sum_{n=1}^{\infty} c_n(t) J_{3/2}(\lambda_n k),$$

where

$$\lambda_n = \frac{a}{2\pi} \omega_n,$$

$\omega_n$ being an increasing infinite sequence of positive numbers generated by the equation

$$J_{3/2}(\omega_n) = 0.$$

These numbers can be well approximated by $(n + 1/2)\pi$, for high $n$ values.

Using (44) in (47) and the orthogonality property of the $J_{3/2}(\lambda_n k)$ functions [14], one obtains

$$c_n + \pi(\omega_n + \omega_n^{-1}) \sum_{n' = 1}^{\infty} \left[ 2E_{nn'} c_{n'} + \omega_E^2 \left( \frac{\omega_n^2}{\pi(\omega_n + \omega_n^{-1})} \delta_{nn'} + A_{nn'} \right) c_{n'} \right] = 0,$$

$$n = 1, 2, \ldots,$$

where

$$E_{nn'} = \left( \frac{a}{2\pi} \right)^2 \int_0^{2\pi/a} E_c(k) k J_{3/2}(\lambda_n k) J_{3/2}(\lambda_{n'} k) dk,$$

$$A_{nn'} = \frac{5}{3} \left( \frac{h}{eE} \right)^2 \int_0^{2\pi/a} A_c(k) k J_{3/2}(\lambda_n k) J_{3/2}(\lambda_{n'} k) dk,$$

and

$$\omega_E = \frac{|e|a}{2\pi h} E.$$

It can now be verified, by direct numerical computations, that, for fields greater than 1 kV/cm, the elements $A_{nn'}$ are negligible quantities in (47). This proves the assertion made in Section 2 regarding the weak contribution of the last term of (14).
Evaluations of (48) show that the diagonal elements are greater (by about one order of magnitude) than the nondiagonal ones. This suggests an iterative approach to the coupled equations (47). However we shall content ourselves, in the present paper, with the zeroth order approximation, i.e. we shall consider the matrix $E_{n'n'}$ as diagonal.

So, if we define

$$E_n = \frac{2\pi^2 \hbar}{|e|a} \pi (\omega_n + \omega_n^{-1}) E_{n'n'},$$

$$\delta_n = \frac{|e|a}{2\pi \hbar} E_n,$$

and

$$r_n = \sqrt{\left[ \frac{E_n}{E} \right]^2 - \frac{3}{5} \omega_n^2},$$

we obtain from (47) the following independent damped oscillator type equations:

$$\ddot{c}_n + (\delta_n^2 - \omega_n^2 r_n^2) c_n + 2\delta_n \dot{c}_n = 0 \quad n = 1, 2, .. ,$$

whose solutions may be easily constructed in order to meet the initial conditions (42) and (43).

$$c_n(t) = -\frac{e^{5/2}}{4V_0} \omega_n^{3/2} \left( \omega_n + \omega_n^{-1} \right) \exp \left( -\frac{\omega_n^2}{4\beta} \right) \exp(-\delta_n t) \times \frac{1}{2r_n} \left[ \exp(r_n \omega_0 t) - \exp(-r_n \omega_0 t) \right].$$

By means of the relations (11), (24), (36), (44) and (55), the electron drift velocity along the field direction becomes:

$$v_d(t) = \frac{4\pi \hbar}{3ma} \sum_{n=1}^{\infty} (-1)^n \sqrt{1 + \omega_n^2} \exp \left( -\frac{\omega_n^2}{4\beta} \right) \exp(-\delta_n t) \times \frac{1}{2r_n} \left[ \exp(r_n \omega_0 t) - \exp(-r_n \omega_0 t) \right].$$

We notice first that the result (56) gives real values, even if some of the $r_n$ numbers are imaginary. Then, the presence of the factor $\exp(-\omega_n^2/(4\beta))$ ensures the absolute convergence of the series. We shall denote by $N$ the number of the significant terms of (56), which is a decreasing “function” of temperature. As an example, for InSb at $T = 77 \, K$, $N$ must be close to 400 to ensure a good precision.

Computations of (51) and (48) showed that the sequence $E_n$ has a complicated $n$-dependence, but this is in quite a narrow interval around a certain mean value. It follows that, for values of $E$ that are not too high, the first few terms in (56) (their number depends on $E$, as one can see from (53)) have an overdamped evolution and the others are “oscillatorally damped”.

It is also evident from (52) that the time extent of the transient response (56) is controlled by the scattering mechanisms through the factors $\exp(-\delta_n t)$.

4. Discussion of the Results

The transient drift velocity given by (56) was computed for InSb using data from the literature [10, 13]. We are only interested in the general problem of the transient response, not in a
Fig. 1. — Transient drift velocity of electrons in InSb calculated at $T = 77$ K for two values of the field strength.

In the particular semiconductor and for this reason we have not included some detailed features such as nonparabolicity and other complications of the band structure.

The main results are presented in Figure 1, where the time variation of the drift velocity is shown for two values of the external field strength, at $77$ K. A high frequency oscillation superimposed on a general overshoot shape may be observed in both cases and its frequency increases with the electric field applied.

From the formal point of view, this behaviour can be explained as follows. The response is expressed as a superposition of a certain number of significant time dependent terms ($N$). This number is determined by the initial conditions and by the temperature, as was shown in Section 3. There are generally three types of response among these terms: the overdamped kind (mainly the first kind), the damped slowly oscillating kind (for intermediate $n$ values in (56)), and the damped high frequency oscillating kind (for $n$ values closed to $N$). The first two types determine the overall shape of the transient response and the last one is responsible for the high frequency oscillations. As can be seen from (53), the greater the applied field, the higher the frequencies of these last terms allowed in the significant set.

From a physical point of view, such oscillations could appear to be the result of the impact of the external field on the electronic system. This produces, first of all, a crowding of the electrons into states of high wave vector along the field direction. The scattering from such states is more effective, deflecting them out of the stream, without important relative variations of the energy. This results in a drop of the drift velocity. If the external field is high enough, it will rebuild the streaming motion before the end of the transient response (whose overall time extent is controlled mainly by the collisions) and new deflections become possible. These phenomena could repeat many times before stationary drift is reached, when a compromise between the field and the scattering is established.

The simple result obtained previously indicates that the scattering mechanisms have a crucial role in the transient response. Indeed, if one computes $v_d(t)$ from (56) by setting the collisions zero ($E_{ac} = E_{po} = 0$), then the curve (a) of Figure 2 is obtained, i.e. a constant acceleration drift (as is intuitively clear).

In addition, if one smooths out the collision operators (i.e. if they are supposed as independent of $k$, this leads to a constant $E_n$ sequence and finally to a result presented as the curve (b)
POSSIBLE GENERATION OF THz DRIFT EFFECTS

Fig. 2. — Transient drift velocity of electrons in InSb calculated for $E = 10$ kV/cm and $T = 77$ K for three particular cases: (a) collisionless (the values of the velocity on the curve should be multiplied by ten); (b) smoothed collision operator; (c) relative enhancement of electron-polar optical phonon interactions.

Fig. 3. — Transient drift velocity of electrons in InSb calculated at $T = 150$ K for the same field strengths as those for Figure 1.

of Figure 2. Here (56) was calculated with $E_n$ equal to its mean value, for the example depicted in Figure 1. A slight overshoot may be observed, but no oscillation appears. This suggests that the scattering might operate a selection among the electrons allowing only some $k$ values to be substantially deflected. When the collisions are smoothed out they cannot distinguish among the $k$ states and are equally effective for all of them, and from the very beginning. This leads to a rapid balance with the external field and so to a stationary drift.

From a formal point of view, the action of the collisions corresponds to a selection operated by the $E_n$ sequence among the terms of (56): it influences both the damping and the amplitude of each term. The absence of such a selection leads to nonoscillatory superpositions of the terms.
as in the cases (a) and (b) of Figure 2.

In order to examine the relative importance of the collision operators in the transient response, the drift velocity was calculated for $E_{\text{ac}}$ diminished by a factor of three and $E_{\text{po}}$ increased by a factor of fifty (the electron-polar optical phonon coupling is relatively weak in InSb [10]). The enhancement of the transient oscillations (Fig. 2c) shows that the electron-acoustical phonon coupling has an inhibitive action on the electronic deflections because of its almost fluid-like damping effect.

Finally the transient drift was calculated for a higher temperature (Fig. 3). As one would expect, given that the electron-phonon interactions are more important and their damping action is more pronounced, the overshoots become smaller and the oscillations weaker.

In conclusion, the simple model used shows that when a high electric field is suddenly applied on a semiconductor, THz transient oscillations could appear as a combined result of the impact of the field on the electronic system and of the selective scattering processes. The effect should be enhanced at low temperatures.

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