Harmonic Solution for Periodic Waveforms of the BTE's for Microwave and Millimetre-Wave Active Device Modelling

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ABSTRACT

A harmonic solution of Boltzmann's Transport Equation (BTE) taking into account its first three moments together with Poisson's equation has been found for a piecewise periodic voltage excitation in a semiconductor. The electric field and potential, density of electrons, electron momentum (or velocity) and electron energy have been discretised in the space domain, and they have been expanded in Fourier series in the time domain. The resulting equation system is clearly non-linear and it is solved by means of a Waveform-Balance technique. The time step is determined only by the required maximum harmonic frequency simply by means of the Nyquist's sampling theory. In this way the relaxation times of the semiconductor is implicitly considered in the analysis. This approach allows for a longer time step than a space- and time-discretised standard solution for many cases of interest.

TRADITIONAL APPROACH

In the traditional time and space-discretised solution of the moments of Boltzmann's equation [1] the discretisation steps must be smaller than a minimum quantity in order to get convergence. For the time variable the step must be sufficiently smaller than the energy, momentum and dielectric relaxation times. This is a major problem when a solution in the microwave or millimetre-wave frequency range is required, because the time step is much smaller than the signal period and the number of time steps becomes extremely large with a very high computing time. A very fine resolution in time is generally not required for the signal analysis, so the number of time steps is unnecessarily large. Closer time steps corresponds to frequency components much higher than the microwave or millimetre-wave frequency band, outside the useful range. Neglecting the time delays of some quantities (e.g. momentum, or energy) we obtain a simpler approach [2, 3]. When their relaxation times are very small compared to the signal period; the time step can therefore be increased. The algorithm however is specific for the application and must be tailored on the individual problem by neglecting the differential term in the suitable equation, and rearranging the system; moreover, in the intermediate region where the time delays are not negligible but still rather smaller than the signal period, the problem remains unchanged.

PROPOSED APPROACH

A different approach has been adopted in our case. The applied excitation is first expanded in Fourier series and are taken into account the firsts *r* harmonics. The space is discretised in a suitable grid and the equations are calculated in these points; given the periodicity in time of the applied excitation, all the quantities (i.e. potential, electron density, velocity and energy) at each position are expanded in Fourier series too, with fundamental frequency as that of the applied signal. The time derivatives are expressed as the exact time derivatives of the Fourier series expansion, whose phasors are computed from (2N+1) samples of in a period (Nyquist's sampling theorem) if N are the number of the desired harmonics. The number of samples in a period, and therefore the correspondent time step, is set with reference only to the maximum frequency of interest, i.e. the maximum between the desired N-th harmonic of the signal and the higher harmonic of the excitation signal. The time derivatives can now be expressed at each time instant for each position in space as a function of the values at the same position at all sampling time instants in the period. Consequently, the equations cannot be solved time instant after time instant as in the case of the traditional time and space

discretisation, since all time samples are present in the equations at each time instant. A consequence is that the Jacobian matrix of the global system in the case of a one-dimensional problem (for all time instants and positions in space) is now (4N+3)-diagonal (39 in the case of N = 9 , i.e. 9 harmonics) for each equation. However the system is solved only once obtaining the solution in all the time discretisation points, while the traditional time-discretised approach requires the solution of a 3-diagonal matrix for each time instant, that usually means a higher computational time and memory occupancy.

RESULTS

Both the traditional, time-space-discretised solution and the proposed time-harmonic-space-discretised solution, have been successfully implemented [4] for a one-dimensional 1μm long homogeneous semiconductor sample with doping density $N_D = 10^{23} m^{-3}$. The diffusion terms have been neglected in the equations for the sake of simplicity in this first phase, while retaining the generality of the approach. Several waveforms with a fundamental frequency from the low microwave to the sub-millimetre-wave ranges have been used to validate the method and to compare the two approaches and the results are practically identical for the two methods, as expected. Here the results for an excitation waveform approximating a square wave are reported. We have used the first five harmonic terms of the Fourier expansion of the square wave, i.e.:

$$v_{(t)} = A_0 + A_1 \cos(2\pi f_0 t) + A_3 \cos(6\pi f_0 t) + A_5 \cos(10\pi f_0 t) \qquad (1)$$

with $A_0 = 0.6V$ the DC component, and $A_n = 2*0.5/(n\pi)$, n = 1..3, the amplitudes for the harmonics. In fig. 1 to 4 the behaviours in a time-space plot of the carriers velocity, their energy, electron density and mobility in two different situations are shown: the fig. 1 and 2 are for a fundamental frequency of 20GHz and the fig. 3 and 4 at 200 GHz. Both situations were been calculated taking into account the contribution of 9 harmonics so time axis is discretised in $Nt = 2N_H + 1 = 19$ points by means of Nyquist's sampling theorem. It is evident the difference of the behaviour of the velocity, carriers density and the energy in the two situations due to the difference of their relaxation times. In fact the energy relaxation time is greater than the velocity one, so at higher frequency, the carrier energy (and mobility) can not follow as well the quick variations of the excitation signal. Both velocity figures shown the "velocity overshoot"
The code is written in C language for a PC and both simulations were made on a Pentium 200 machine. The solution requires a computing time of 32s in the first case with 12 iterations, and 27s in the second case with 11 iterations. The robustness of the algorithm was been proved for different wave shapes (ex.: rectangular, triangular, ..) showing a very good convergence, speed and reliability.

Bibliography

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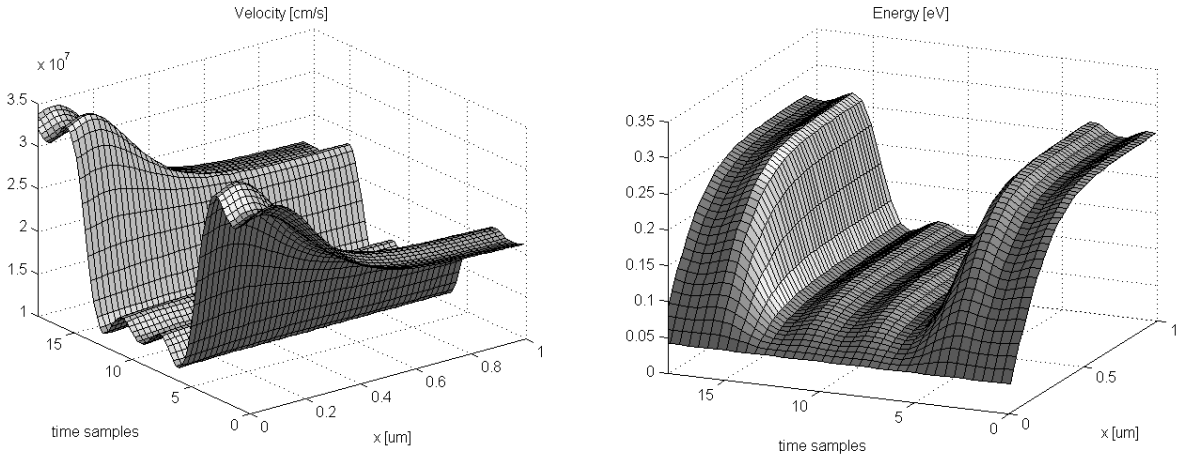

Fig.1 Electron velocity (left) and energy (right) as a function of time and space for an approximated square wave with a fundamental of 20 GHz

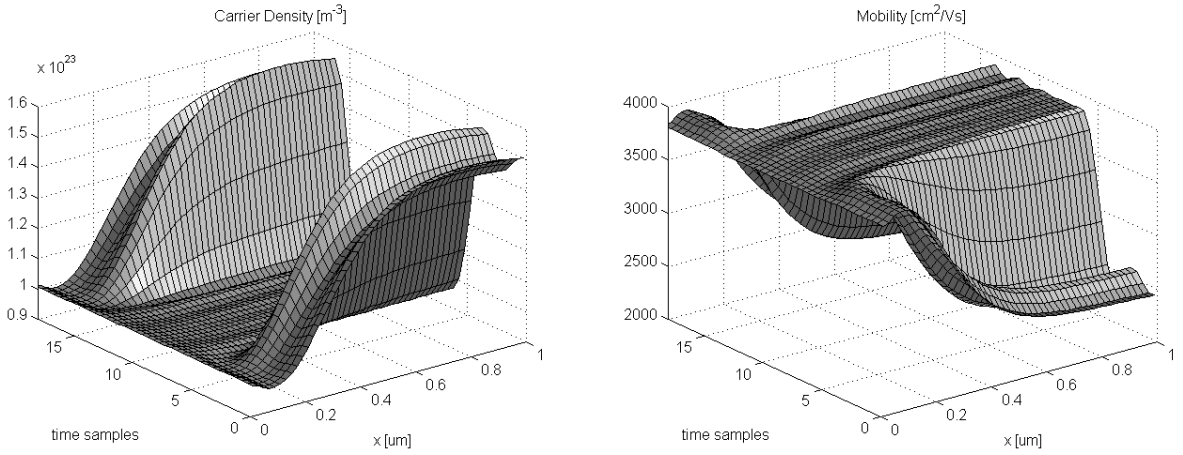

Fig.2 Electron density (left) and mobility (right) as a function of time and space for an approximated square wave with a fundamental of 20 GHz

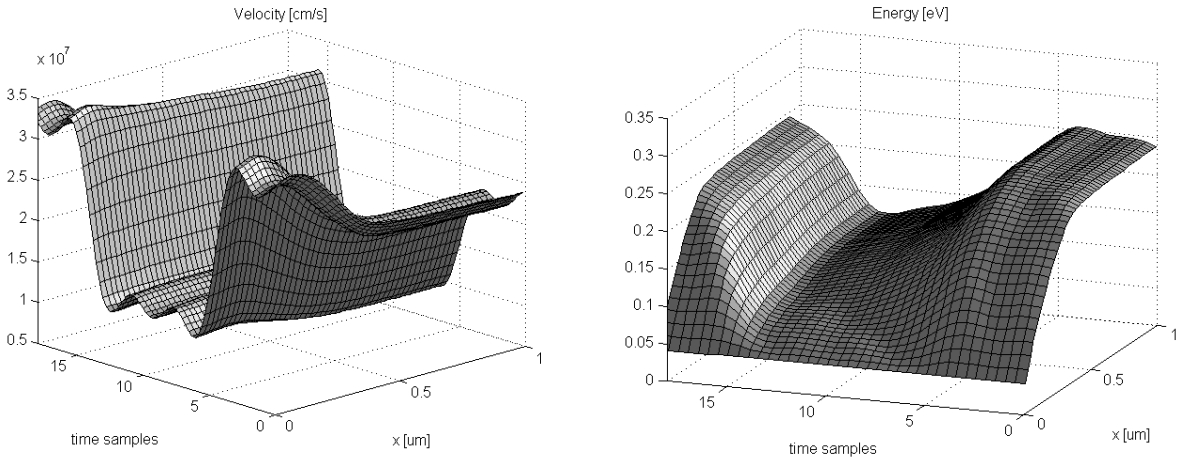

Fig.3 Electron velocity (left) and energy (right) as a function of time and space for an approximated square wave with a fundamental of 200 GHz

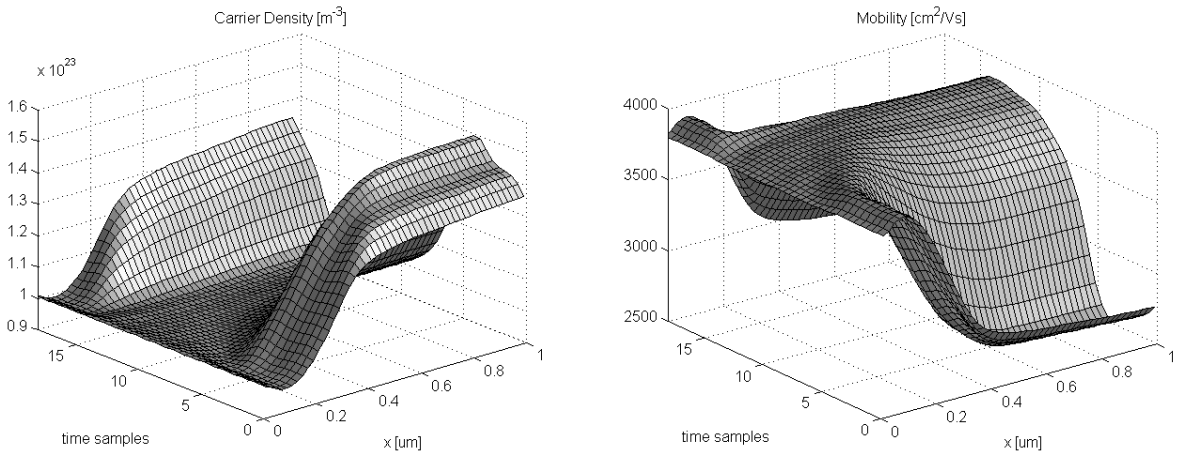

Fig.4 Electron density (left) and mobility (right) as a function of time and space for an approximated square wave with a fundamental of 200 GHz