Monte Carlo Simulation of S-Type Negative Differential Conductance in Semiconductor Heterostructures

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Abstract

Within an ensemble Monte Carlo method, we simulate a bipolar transport in a vertical layered *n*-GaAs/*n*-AlGaAs/*i*-GaAs heterostructure placed between n^+ and p^+ contacts. A very fast switching time and, hence, a very high frequency (up to 1 *THz*) of the voltage oscillations are predicted.

1. Introduction

Solid-state devices with S-type current-voltage characteristics have a wide application as fast switchers and microwave power generators. In recent years, significant attention has been payed to the heterostructure hot-electron diode (HHED) [1] based on the multilayer n^+nn^+ GaAs/AlGaAs structure. From both an experimental and theoretical analysis, this structure is found to exhibit S-type negative differential conductance (NDC) and high-frequency oscillations up to 100 GHz at temperatures below about 77 K [1,5]. To improve its high-frequency performance, we propose the replacement of the anode n^+ contact with a p^+ layer, thus introducing the possibility for an additional hole current and for a switching which occurs between the low-conductance state associated with the hot-electron current and the high-conductance state associated with the hot electron-hole current.

2. Model

We consider the vertical transport in a layered heterostructure which consists of an active region placed between heavily doped GaAs n^+ and p^+ contacts. The active region contains three layers: A, B and C. The *n*-GaAs layer A is placed at the n^+ contact and serves as a drift region for electrons and holes. The switching time and

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generation frequency depend mainly on the length of this layer. The n-AlAs layer B creates a barrier of about $0.53 \ eV$ for holes. Because of the high resistivity of AlAs, as compared with GaAs, the B layer must be as thin as possible. The undoped GaAs layer C (spacer) is introduced between the B layer and the p^+ contact to minimize the dispersion in energy of the momentum distribution of holes entering the hole barrier. As found from Monte Carlo (MC) simulations, the best device performance is obtained when the C layer thickness is of about $100 \div 300$ Å. Another important parameter is the thickness of A-B and B-C heterojunctions. Again, simulations show that abrupt junctions are undesirable for the proposed device due to their high junction-capacitance, while $20 \div 100$ Å wide junctions are more suitable. We take the junction region formed by $Al_xGa_{(1-x)}As$ where x changes monotonically from 0 to 1 with distance. All the results we shall present in the following are obtained for a structure with an active region length of 1700 Å. The length of the layer A is 1500 Å, and the doping concentration is $n = 1.5 \times 10^{17} \text{ cm}^{-3}$. Both layers B and C are 100 Å thick, with doping concentration of $n = 1.5 \times 10^{17} cm^{-3}$ and no-doping, respectively. The thickness of the A-B and B-C heterojunctions is assumed to be the same and equal to 40 \mathring{A} . The doping concentration of contacts is $n^+ = p^+ = 5 \times 10^{19} \ cm^{-3}$. The energy-band diagram of the proposed structure is schematically shown in Fig. 1. The graded heterojunctions enables us to smooth the discontinuity steps of the potential (or energy) at the heterojunction. Under these conditions, carrier tunneling through the potential barriers is neglected in favour of classical thermionic process. The carrier transport throughout the structure is theoretically investigated making use of a direct solution of the coupled Poisson and Boltzmann equations obtained with a MC technique. A three-valley conduction band and a single heavy-hole valence band is considered with spherically symmetric nonparabolic dispersion laws in all bands. The lattice temperature is assumed to be 300 K.

3. Results

The peculiarity of the structure is that layers A and C serve as heating regions for electrons and holes, respectively, and the intermediate layer B is the place where potential barriers prevent electrons and holes from penetrating into the diode. Figure 2 reports the current-voltage characteristics of the whole structure calculated under dynamical conditions [6]. At the lowest applied voltages both barriers act as closed gates and the system is in the lowest conductance-state. At increasing voltages, a first high conductance-state is achieved when the electron barrier acts as an open gate owing to thermionic emission of electrons via upper valleys. By further increasing the voltage, the onset of a second higher conductance-state, which corresponds to the situation where also the hole barrier acts as an open gate, takes place. The above three states (labelled respectively as I, II, and III) give rise to a conductance which is controlled, respectively, by a cold electron, a hot electron and a hot electron-hole current. The switching from one state to another is responsible for a large variation of the total current at practically the same applied voltage which, in turn, should lead to the appearance of S-type regions in the current-voltage characteristic. The simulation of the current transport throughout the given structure shows that the transition between states I and II does not lead to an S-type NDC, while the transition between states II and III is accompanied by a strong S-type behavior. This last behavior is further enphasized when the structure is connected in series with a load resistance R and in parallel with a capacitance C. Figure

3 shows the time variation of the voltage drop between the terminals of the load resistance, $U_{R}(t)$, when a voltage pulse $U_{a}(t)$ is applied to the whole circuit. The value of R is $10^{-11} \Omega m^2$ and $C = 200 C_d$, where C_d is the geometrical capacitance of the structure. The fast switching of $U_R(t)$ (with switching time t_{on} less than 10 ps) is independent from the sweep of $U_a(t)$. To clarify the switching mechanism, the evolution of the potential drop on the layer A, $U_A(t)$, and the average concentrations of electrons in the X-valley, $n_X(t)$, and holes in the layer A, p(t), are presented in Fig. 4. Both $n_X(t)$ and p(t) values are normalized to the average concentration of electrons in the layer A. The fast growth of $n_X(t)$ for $U_A(t) > 0.5 V$ is associated with the onset of thermionic emission of electrons over the barrier or, in other words, to the I-II transition. The further increase of $U_A(t)$ is followed by a slow increase of the electron current which is typical in short n^+nn^+ structures. When the current becomes sufficiently large to create a voltage drop on the C region high enough for holes being able to overcome the barrier, the II-III transition starts, i.e. p(t) increases from 0 to 1. The rise-time of p(t) corresponds approximately to t_{on} . Obviously, for the realization of such an effect, at the hole barrier the dispersion in energy of the hole momentum-distribution in the field direction must be much less than the barrier height. The simulation shows that t_{on} of $1 \div 2 ps$ can be obtained at 77 K. Under current-driven operation, the structure exhibits an oscillatory behavior in a certain range of current values. Figure 5 shows the voltage oscillations between the diode terminals when a constant total-current $j_{tot} = 3 \times 10^{10} A/m^2$ is flowing through it. The voltage oscillates because of the periodic transitions between states II and III of the structure. The correspondig frequency of the oscilltions, 220 GHz, well correlates with a switching time of about 10 ps. Our simulations show that the terahertz frequency range can be achieved at lattice temperatures below about 77 K.

In conclusion, we have proposed a new heterostructure which, according to MC simulations, can operate as a switcher with switching times less than 10 ps. The switching mechanism is based on the fast transition from a low to a high conductance state which can occur under vertical transport. The heterostructure can be also used as a microwave generator with characteristic frequencies higher than 200 GHz. At temperatures below about 77 K the switching time can be reduced to values below 1 ps, thus implying oscillation frequencies in the THz region.

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Fig. 2 - Current-voltage characteristic of the whole heterostructure obtained from a Monte Carlo simulation by taking a linearly-small increase with time of the total current j.



Fig. 4 - Time variation of the voltage drop at layer A , and of the average concentrations of X-valley electrons and holes in the layer A (respectively, curves 1 to 3).

Fig. 1 - Schematic representation of the energy-band diagram of the active part of the heterostructure which consists of $0.15 \ \mu m \ n - GaAs$ (layer A), $0.01 \ \mu m \ n - AlAs$ (layer B) and $0.01 \ \mu m \ i - GaAs$ (layer C). Solid, dashed and short-dashed lines correspond, respectively, to the Γ , L, and X-valleys of the conduction band. Dotted line shows the valence band edge.



Fig. 3 - Time variation of the voltage applied to the whole circuit (curve 1) and of the voltage drop between the the terminals of the load resistance (curve 2).



Fig. 5 - Time oscillations of the voltage drop between the diode terminals calculated under constant-current operation.