Monte Carlo Simulation of transport in two-dimensional electron gas via energy relaxation

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***Abstract*— We simulated the process of energy thermalization in two-dimensional-electron-gas (2DEG) via electron-electron scattering by Ensemble Monte Carlo (EMC) method. Time evolution of electron energy distribution indicates that the response of electrons, in terms of energy distribution, in 2DEG to external perturbation is at sub-picosecond time scale. By applying the results to the physcial model of our device, we successfully explain previous experimental results of photodetectors showing speeds higher than response times, faster than those limited by transit time.**

I. Introduction

Planar Metal-Semiconductor-Metal(MSM) photodetectors [1] have been widely applied in optical communications and opto-electronic integrated circuits (OEIC) for their excellent performance and compatibility with integrated circtuis (IC) processing. We have fabricated 2DEG based MSM photodetectors [2], on the same structure as HEMT, but with Schottky contact for anode and cathode. The dynamic response of such a device should be dependent on transit time, which is determined by contact separation. However, we have observed similar Full-Width-Half-Max (FWHM) time responses for contact sparation of 2 and 4 μm devices [2], both around 10 ps. Importantly, these responses have been faster than that which is allowed by the transit time of carriers.

Detailed static simulation of the device structure have been carrierd out by ISE-TCAD software, showing a vertical orientated electric field and high density of confined mobile carriers [3], which indicates the transit time of photogenerated carriers consisting of time of vertical transit through the absorption region and time of latteral transport along the 2DEG. We performed the dynamic simulation based on Ramo's thereom in the absorption region for the former and Monte Carlo simulation in the 2DEG for the later. Combining both enabled a successful explaination of our experimental results, provided that electrons rearrange their energies before real charge transport occurs. The rearranged 2DEG subsystem relaxed as a whole by carriers are swept to the the external circuits, thus inducing the photocurrent.

In this article, we will describe the detailed Monte Carlo simulation regarding the dynamics of electron transport in 2DEG. The assumptions and procedures will be addressed with formulation and implementaion. It will be followed by a discussion of applying the result to our physical model of the device, and eventually lead us to the full understanding of the device behavior.

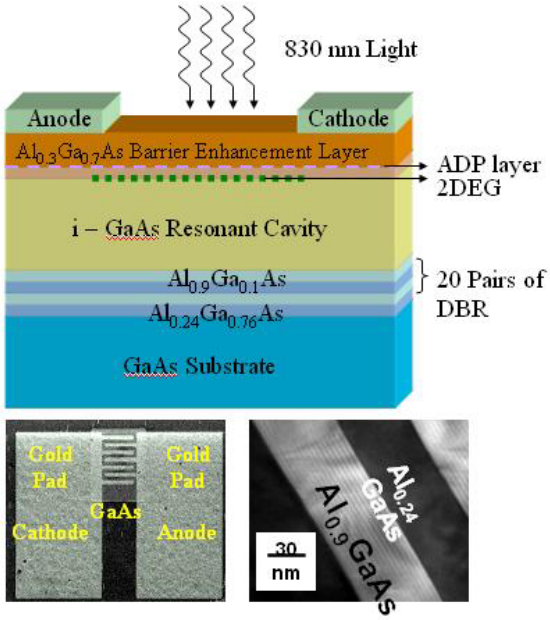

Fig. 1. Schematic layer structure of photodetector. The lower-left picture is the SEM of the top view of the interdigitated metal contacts. The lower-right is a image TEM of one pair of DBR structure Dense 2DEG exists at the hetero-interface.

II. Simulation and Results

A. Device Structure

We previously fabricated a GaAs-based, δ-doped Heterostructure MSM with a resonant cavity and a Distributed-Bragg-Reflector(DBR) by molecular beam epitaxy (MBE) [2]. The layered structure is shown in Fig.1. $Al_{0.9}Ga_{0.1}As/Al_{0.24}Ga_{0.76}As$ DBRs were grown on a 200 nm GaAs buffer layer, with the thicknesses of each layer being 67.6 nm and 59.6 nm respectively. Above the DBR was a 117.5 nm undoped GaAs a resonant cavity. The absorption region followed by a 50 nm thick $Al_{0.3}Ga_{0.7}As$ barrier enhancement layer. An atomic planar Si-doped δ layer was grown with the sheet density of $5x10^{12}$ between barrier and a undoped spacer layer of 5 nm thick. The top contact was deposit with finger width of 2 μm and spacings of 2 or 4 μm.

The device has been reported with high wavelength selectivity at 850 nm, and low dark current of a few tens of picoamperes. High speed time response measurements found

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the full-width-at-half-max(FWHM) were 10.6 ps and 10.7 ps for finger gap of 2 and 4 μm respectively, which were much faster than devices of equivalent dimensions.

The simulation of dynamic transit through the absorption region has been been performed by Ramo's theroem. We further employed the emsemble Monte Carlo (EMC) method to simulate the photogenerated electrons transport along 2DEG after arriving in the 2DEG by following the vertical electric field.

We established a model for 2DEG for the purpose of EMC simulation. An equilibrium 2DEG was subject to Fermi-Dirac energy distribution at room temperature. A small amount of electrons, which emulate the photogenerated electrons arriving the 2DEG, are introduced with a Gaussian energy distribution. The mean value of energy is 150 meV above the average energy of the 2DEG in equilibrium, considering the extent of conduction band bending in the absorption region. By observing the evolution of the energy distribution function of the 2DEG as a whole, we are able to find out the electron thermalization time in the 2DEG.

B. Electronic States

To incorprate the quantum effects in 2DEG, it is necessary to find out the electronic states of the triangular-well, which basicly are quantized subband energy levels and the corresponding wave functions indicating electron density distribution. The quantized energy levels are proportional to the inverse cubic root of the effective mass. Since the effective masses in the subsidiary valleys are larger than in the Γ valle, size quantization effects are small in the L or X valleys. Therefore, we account for size quantization effects only in the Γ valley. An uniform effective mass of $0.067m^*$ and dielectric constant of 12.9 are used in both GaAs and AlGaAs layers.

The routine was performed by self-consistent numerical solution of Possion's equation and Schrödinger's equation [4]. The wave function $F_m(z)$ normal to the layer interface for the m-th subband, satisfies the following Schrödinger equation:

$$-\frac{\hbar^2}{2m^*}\frac{d^2F_m(z)}{dz^2}+V(z)F_m(z)=E_mF_m(z) \qquad (1)$$

The effective potential energy $V(z)$ is given by

$$V(z)=-e\phi_e(z)+V_h(z)+V_{xc}(z) \qquad (2)$$

where, $\phi_e(z)$ is the electrostatic potential given by the possion equation below. V_hz is conduction band offset, $V_{xc}(z)$ is the local exchange correlation potential. The Poisson's equation is given by,

$$\frac{d^2\phi_e(z)}{dz^2}=\frac{e}{\epsilon_0\epsilon}[\sum N_i{F_i}^2(z)+N_a(z)-N_d(z)] \qquad (3)$$

where N_i represents the number of the electrons in the subband i and is given by

$$N_i=\frac{m^*k_BT}{\pi\hbar^2}ln[1+exp[\frac{E_F-E_i}{k_BT}]] \qquad (4)$$

The Schrödinger equation can be solved using Numerov method [5]. We start with a trangular well, find the energy state and wavefunction for each state. We take the first three subbands, and the charge distribution can be calculated by summing up all three subbands for potential evaluation in Poisson's equation. The calculation converges after several iterations, and the first three subbands are 55.5 meV, 97.6 meV, and 119.9 meV above the minimal of the conduction band respectively.

Our treatment of the 2DEG involved a high concentration of electrons, where degeneracy is expected to play an important role. We also include the rejection technique to account for the Pauli exclusion principle in the EMC technique. With the EMC technique, the distribution function evolves with the ensemble and is known at every instant of time. Once the final state is selected, during the transient phase, a random number between 0 and 1 can be used to accept or reject the transition. As the procedure is iterated, a steady state will eventually be reached with the probability of transitions into the state proportional to the occupancy of that state.

C. Electron-Electron scattering

Our EMC only considered electron-electron scattering in 2DEG sinnce the electron-electron scatering rate is much larger than that of electron-phonon scattering [6], which is the dominant energy dissipation mechanism in the GaAs channel at room temperature. The e-e scattering rate in bulk material has been previously calculated using the Born approximation [7]. We start by considering the scattering rate between an electron in the well with wave vector k in subband i and a second electron with wave vector k_0 in the subband j. The final states of these two electrons are k' and m for the first electron and K_0' and n for the second electron. The total scattering rate is given by

$$\Gamma_{im}(k)=\frac{4\pi e^4m^*}{\hbar^3Ak^3}\sum_j f_j(k_0)\int_0^{2\pi}d\theta\frac{|F_{ijmn}(q)|^2}{(q+q_{s0})^2} \qquad (5)$$

where $f_i(k_0)$ is the disribution function, $F_{ijmn}(q)$ is the form factor, given by

$$F_{ijmn}(q)=\int_{-\infty}^{\infty}dz\int_{-\infty}^{\infty}dz'\phi_i(z)\phi_j(z')\phi_m^*(z)\phi_n^*(z')e^{-q|z-z'|} \qquad (6)$$

where, $\phi_i(z)$ is the wavefunction at the i-th subband.

The e-e scattering was included into the MC simulation using a modification of the self-scattering technique [8] for the bulk. Here we take the full multisubband scattering rate and the maximizing function that is integrable, calculate the total scattering rate, and account for the actual value of the function when the final state is chosen through a rejection method. For the intrasubband scattering rate, we note that the integrand is sharply peaked at $q=0$ corresponding to $\theta=0$ and 2π. Since the formfactor is always less than unity, the maximum value of the integrand is always less than $1/q_0^2$. Thus the maximum scattering rate is given by

$$\Gamma_{max,ii}=\frac{4\pi^2e^4m^*N_s}{\hbar^3k^2q_0^2} \qquad (7)$$

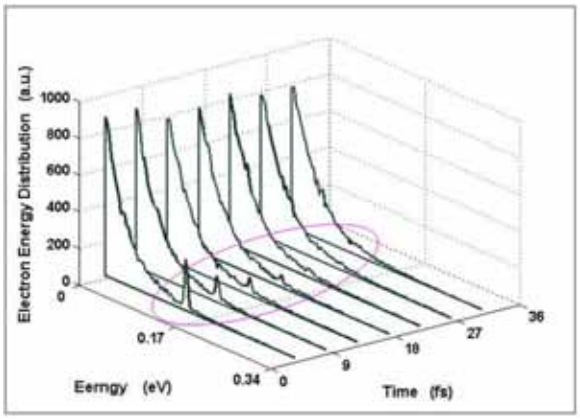

Fig. 2. Monte Carlo simulation shows the time evolution of the energy distribution in 2DEG when perturbed by extra electrons with energies above average. the peaks in the oval are the extra electrons; redistribution is achieved in tens of femto-secondss

where N_s is the total sheet density of the QW.

In the beginning of the scattering, an electron is chosen at random from the emsemble, and the scattering angle is chosen at random according to the flat distribution associated with the maximizing function. Using another ramdom number between zero and the maximum value of $1/q_0^2$, the actual value of the integarnd is compared to that of the ramdom number, the scattering is rejected if the integrand is less than this number. In this case, the electron and its counterpart are then allowed to continue their free flight. If it is less than the integrand value, then the scattering is accepted, the momentum and energy change accordingly.

The scattering event is calculated for each electron for each time step, and the time step is chosen such that there are a decent number of scattering event occuring in each step. After each step the electron energy distribution rearranges itself, and eventually reaches a steady state.

D. Simulation results

The time evolution of electron energy distribution is calculated and shown in Fig.2. Each curve represents a energy distribution function at some time.

We clearly observe from the Monte Carlo simulation that the 2DEG under perturbation could reach a quasi-equilibrum state with an elevated quasi-Fermi level in a few tens of femtoseconds, which is consistent with the experimental results performed by Bell labs [9].

III. Discussion

Given the electron thermalization time at the femtosecond level, we consider that the 2DEG system relaxes to thermal equilibrium in such a small time that the transport time in 2DEG becomes negligible compared to the transit time in the absorption region. During this time, the Fermi level of the 2DEG subsystem is elevated to a quasi-Fermi level, which is higher than the former device Fermi level, and falls when the new equilibrium is established between system and the 2DEG after the electrons under the anode were swept to the contacts.

This is a continuous process that carriers are swept to the contacts as long as the quasi-Fermi level is above the system Fermi level. It can be interpreted that the electrons under anode are affected by the energy variations of any other electrons in the 2DEG in a few tens of femtosecond by sensing the elevated quasi-Fermi level. In another words, energies of electron travel through the 2DEG in a much smaller time than the real electrons transport. This results is intuitively reasonable since electron-electron scattering is an inelastic dynamic scattering process, which is the most efficient channel of energy swap in two-dimensional electron system.

In this manner, 2DEG could work as an extended contact, more specifically anode, to collect electrons. The simulation reaults also justify the case when electrons were injected with less energies, which should take less time to equilibrate with 2DEG.

IV. Conclusion

In conclusion, we have simulated the electron transport in 2DEG by EMC method. A sub-pecosecond energy relaxation time was achieved, which suggests a response time of the device only subject to the transit time in the absorption region. The extremely fast electron energy thermalization, benefited by the two blocking Schottky contact, circumvents the drift limitation of electron drift transport, and could be applied in a wide range of high speed device design.

Acknowledgment

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