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Analysis of Conditions for Free-Carrier Grating Formation in InP n^+nn^+ Structures using Monte Carlo Technique

V. GRUŽINSKIS, P. SHIKTOROV AND E. STARIKOV

Semiconductor Physics Institute A. Goštauto 11, LT-01108, Vilnius, Lithuania

Electron transport in 5 μ m long InP n^+nn^+ structure with the *n*-region doping of 10¹⁵ cm⁻³ is theoretically investigated by the Monte Carlo particle technique at low lattice temperature (T = 10 K), when dominating scattering mechanism is the optical phonon emission. It is shown that at the constant bias a free-carrier grating can be formed inside the *n*-region. The free-carrier grating formation conditions are analysed by Monte Carlo particle simulation of electric field profiles and noise in the considered InP structure.

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1. Introduction

Recently the modelling of electron transport in indium nitride based long (of few μ m) n^+nn^+ structures, when optical phonon emission is dominating scattering mechanism, shows the possibility of the cyclic real-space motion of carrier ensemble which leads to the formation of free-carrier grating (FCG) in the *n*-region of the biased structure [1]. At a proper bias and doping conditions the THz radiation from InN structure with the FCG is possible [1]. The microwave generation appears near the frequency, which is reciprocal to the transit time between adjacent FCG maxima.

The aim of this article is to analyse the conditions for the FCG formation in InP n^+nn^+ structures.

2. Model

The calculations of electron transport in n^+nn^+ InP structures are performed by simultaneous solution of coupled Boltzmann and Poisson equations by Monte Carlo particle technique [2]. The InP band and material parameters of a spherically symmetric nonparabolic conduction band are taken from Ref. [3]. Electron scatterings by polar optical and acoustic deformation phonons, and ionized impurities are accounted for. Due to relatively high electron heating up to energies of 20–50 meV the acoustic scattering is considered as elastic one. The doping of simulated 0.02–5–0.02 $\mu m n^+nn^+$ InP structure is $n = 10^{15}$ cm⁻³ and $n^+ = 10^{17}$ cm⁻³. The calculations (if not indicated) are made for lattice temperature T = 10 K. The number of simulated particles and the time step in all cases is of 3.6×10^5 and 5 fs, respectively.

3. Numerical results

As a first step the current-voltage relation (CVR) of InP structure is simulated by MCP technique. At the given bias the current response is simulated until the stationary behavior of current j(t) is achieved. The time average of stationary part of j(t) is chosen as a current point at the given bias. The interval between so calculated bias points is of 0.01 V. The small interval between bias points allows us to reveal the CVR pecularities at low voltages (see Fig. 1a).



Fig. 1. (a) Current–voltage relation of the InP structure. The arrows 1 and 2 denotes the bias points at which electron can gain energy of 1 and 2 optical phonons, respectively, during the flight over entire *n*-region. (b) The simulated stationary parts of currents j(t) in InP structure at the biases U = 0.02, 0.035, 0.045, 0.09, 0.2, 0.4, and 0.6 V (curves from bottom to top, respectively).

In Fig. 1a the humps can be well recognized at the biases $U = u_0$ and $2u_0$, where $u_0 = \hbar\omega_0/e$, $\hbar\omega_0$ is the optical phonon energy (0.043 eV for InP), and e is the electron charge. The humps are caused by the current oscillations (see Fig. 1b) due to the plasma instability (PI) [4]. The oscillatory behaviour of current manifests itself in the bias range from $U = u_0$ up to U = 0.6 V (Fig. 1b). The lower bias limit $U_{l0} = u_0$ for current oscillations due to the PI is conditioned by the onset of optical phonon emission process at $U > u_0$ while the upper current oscillation limit U_{up} is of about 0.6 V (see Fig. 1b) and is related to the FCG formation at suppressed PI conditions. To analyse the FCG formation conditions the profiles of electric field E(x) and local optical phonon emission rate $\nu_o(x)$ in *n*-region of InP structure are simulated and presented in Fig. 2a,b.



Fig. 2. The profiles of electric field (a) and local optical phonon emission rate $\nu_0(x)$ (b) in the *n*-region of InP structure at the different biases U.

All the profiles are obtained by averaging the instant distributions over the time much longer than j(t) oscillation period. The simulated electric field profiles are demonstrated in Fig. 2a. The essentially nonuniform field distributions are evident. At $U < u_0$ all the field is concentrated near the cathode and in the rest of *n*-region it is close to zero (see solid curve in Fig. 2a). Such a field distribution is similar to that at the ballistic transport conditions [5]. When the bias is $U > u_0$ the enhanced field region appears near the anode contact and it widens at the increased bias. The enhanced field is formed in the regions where the electrons emit the optical phonons (compare Fig. 2a and b). At the bias U > 0.25 V the FCG is formed in the *n*-region of the InP structure due to periodic motion of the electrons under optical phonon emission, Fig. 2a. The most regular FCG is formed in the bias range 0.3 < U < 0.8 V. At U > 0.8 V the field profile in the *n*-region turns to the monotonically increasing with coordinate modulated field distribution. The analytical FCG model [1] with only optical phonon emission accounted for gives the minimal bias for FCG formation in given structure $U_{\min} = 0.565$ V. This means that for the given structure at the quasiballistic transport conditions the FCG will be not formed at $U < U_{\min}$. It is confirmed by simulations of the given structure with only optical phonon emission accounted for.

In the real structures with all main scattering mechanisms accounted for the grating formation starts at the biases less than U_{\min} (see Fig. 2a). The scattering by accoustics phonons and ionized impurities suppresses the PI which prevents the grating formation. Also the PI is suppressed at elevated temperatures due to the widening of electron distribution in velocity space and enhanced scattering by accoustic phonons and optical phonon absorption at higher temperatures. In Fig. 3a three simulated electric field profiles at U = 0.2 V are shown: curve 1 corresponds to the conditions of Fig. 2a, curve 2 is simulated at increased impurity scattering, and curve 3 is simulated at elevated temperature. One can see that the suppressed PI allows the FCG formation (curves 2 and 3 in Fig. 3a).

It is well known that current oscillations give the current noise enlargement in some frequency regions [6]. Therefore, the current noise is simulated using the MCP technique [6]. The simulated current noise spectral densities for the considered InP structure are presented in Fig. 3b. One can see in Fig. 3b that high noise level at the onset of optical phonon emission (U = 0.045 V) is highly suppressed at U = 0.8 V.



Fig. 3. (a) The profiles of electric field in the *n*-region of InP structure at U = 0.2 V. Curve 1 is simulated at the conditions of Fig. 2a, curve 2 is simulated when the impurity concentration 5 times exceeds the electron concentration in *n*-region, curve 3 is simulated at T = 80 K. (b) Simulated current noise spectral densities of InP structure at different biases U.

The simulation of given InP structure in external resonant circuit as in the case of Ref. [1] gives the microwave power generation at U = 0.3, 0.4 and 0.5 V in the frequency ranges 0.25–0.31, 0.34–0.42, 0.4–0.5 THz, respectively.

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