Simulation of a THz radiation source on AlGaAs/GaAs superlattices

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Abstract. We report on the results of simulations of the carrier transport processes in THz radiation sources. The current-voltage characteristic, dipole matrix elements and LO-phonon relaxation time were obtained using the Ensemble Monte Carlo method, the shooting and effective mass methods. The electron-longitudinal phonon interaction assumed as a dominant mechanism of the carrier scattering for the current-voltage characteristic. The weakly coupled AlGaAs/GaAs superlattices considered for simulations.

1. Introduction
Light emitting devices based on semiconductor superlattices nowadays have a broad range of applications: from medical diagnostics up to optical communication systems. First ideas of a light emission phenomenon in the semiconductor superlattices based on the intersubband transitions were proposed by R. Kazarinov and R. Suris in 1971 [1] and implemented in the first quantum cascade laser (QCL) by a group of researchers led by F. Capasso in 1994[2]. Since then the QCL production has expanded and enhanced, but challenges such as the development of THz radiation sources remain to be accomplished. In order to improve device in the early stages of the development, computer simulations might be applied to predict operational characteristics. One of the most valuable applications of simulation is computing current-voltage characteristics and dipole matrix elements of the structure of a device.

In this research, the Monte Carlo, shooting and effective mass methods are used. The weakly coupled semiconductor superlattices were considered as the initial design for THz sources due to the fact that they experimentally demonstrate negative differential conductivity regions on their current-voltage characteristics. Two types of GaAs/AlGaAs superlattices (Table 1) with doping $5 \cdot 10^{14} cm^{-3}$ were investigated at temperature 65 K. The current-voltage characteristic, dipole matrix elements and LO-phonon relaxation time were obtained.

Table 1. The GaAs/AlGaAs investigated structures description.

| Structure # | Barrier thickness, nm | Well thickness, nm | Al fraction in AlGaAs, % |
|-------------|-----------------------|--------------------|--------------------------|
| 1           | 1.5                   | 18.1               | 10                       |
| 2           | 2                     | 10                 | 30                       |
2. Calculations methods

The carrier transport is assumed as a sequence of transitions of electrons between energy states. Therefore, an initial stage of the simulation technique is to obtain eigenvalues and eigenvectors, i.e., a numerical solution of Schrödinger-Poisson equation system for a given conduction band profile. For this matter, the shooting and effective mass methods applied. At the second stage, the scattering rates are calculated. In a particular case, only two dominant scattering mechanisms are considered for THz radiation sources:

- electron-longitudinal phonon (LO) interaction;
- electron-electron scattering.

The theory of scattering on LO phonons is introduced with the Frohlich Hamiltonian and using the Fermi’s golden rule the phonon lifetime obtained (Figure 1b) as the following [3]:

$$\tau_{ij}^{-1} = \frac{m^*e^2E_{LO}}{2\hbar^3\varepsilon_p} \int_0^{2\pi} \frac{dzdz'\psi_i(z)\psi_j(z)e^{-q|z-z'|}\psi_i(z')\psi_j(z')}{Q} d\theta,$$

where $E_{LO}$ is the LO phonon energy, $m^*$ electron effective mass, $Q$ phonon wavevector, $\psi_i$ a wavefunction for the energy state with index $i$, $\varepsilon_p$ relative permittivity. The numerator of (1) also referred to as a form-factor $F(Q)$.

Electron-electron scattering can be considered in two ways:

- screened Coulomb potential (short-range interaction);
- electron-plasmon coupling (long-range interaction).

The second one will be neglected, due to the fact that it becomes significant only at higher doping levels. Considering electron-electron scattering as a two-electron process, the scattering rate can be written in the form [4]:

$$W_{ik,j} = \frac{m^*e^2}{32\pi\hbar^3\varepsilon_0} \sum_i f_{i_0}(k_0) f_{i_0}(k_0) \int_0^{2\pi} \frac{d\theta}{(q+q)^2} |F_{i_0j_0}(q)|^2,$$

where $q = k - k'$ and $k$, $k'$ – initial and final wavevectors of an electron, $k_0$ – init. wavevector of the second electron, $q_0$ – screening wavenumber in the approximation of single band [4], $f_{i_0}(k_0)$ – carrier distribution function, $i, j$ – initial and final subband numbers of the first electron, $i_0, j_0$ – of second electron, $\theta$ – angle between $k_0 - k$ and $k_0' - k'$.

The form-factor defined in a slightly different way:

$$F(q) = \left| \int_{-\infty}^{+\infty} dz \int_{-\infty}^{+\infty} dz' \psi_i(z)\psi_{i_0}(z')e^{-q|z-z'|}\psi_j^*(z)\psi_{j_0}^*(z') \right|^2.$$

The second electron is chosen randomly from the ensemble during the scattering simulation process. In (2) the 1/2 factor was introduced to consider only the interaction of electrons with antiparallel spin since it prevails over the interaction between electrons with parallel spin.

The derived values of scattering rates considered in the third simulation stage that exploits the ensemble Monte Carlo (EMC) method, i.e., statistical sampling of the scattering events for a large ensemble ($N_e = 10^5$) of carriers [4]. The EMC method considers periodic boundary conditions, which implies simulation of the scattering between states of the central and two nearest periods. The scattering event from one state to the other was simulated using a pseudo-random generator that exploits normalized probabilities of the scattering.
3. Results and the proposed structure

![Graph](image)

**Figure 1(a, b).** (a) Dipole matrix elements of structure 1; (b) The LO-phonon lifetime for $k_{\text{init}} = 0$. $L$ – the width of the well, $F$ – field applied to the structure, $d$ – the thickness of the structure.

The first structure - the superlattice proposed in the literature [5] used as the benchmark for the simulation methods. Its dipole matrix elements (Figure 1a) exhibit the resonance behavior for transitions with tunneling through one and two quantum wells near 10 kV/cm. The dipole matrix elements remain high even beyond resonance regions, which is in the good agreement with the different theoretical approach [5].

The LO-phonon lifetimes (Figure 1b) were calculated for different width of the well. The relaxation time increases with the field due to the increase of transition and LO-phonon energy difference, that weakens scattering rate through $Q$ in (1). The demonstrated behavior was also suggested in previous theoretical consideration [3]. The obtained current-voltage characteristic (Figure 2a) exhibits satisfactory agreement with experimental data. The obtained results demonstrate plateau regions similar to the experimentally observed.

![Graph](image)

**Figure 2(a, b).** (a) Simulation results and experimental data of current-voltage characteristic of structure 2. The arrows emphasize plateau areas; (b) Simulation results for spectral gain.

The second structure is the proposed structure of a THz radiation source. For the described structure the transition occurs between first energy level and second energy level through three quantum wells. For this transition to happen the barriers of the structure shall be weak. The weakness of barriers implies reasonable barrier thicknesses and low amount of Aluminum fraction. The latter is
also important for obtaining less strained structures. The new design demonstrates sufficient gain for the wavelengths near expected transition (Figure 2b).

4. Conclusion
We described simulation techniques for GaAs/AlGaAs superlattice investigation. Obtained dipole-matrix elements, LO-phonon lifetimes show good agreement with theoretical estimations proposed earlier and current-voltage exhibit satisfactory agreement with experimental data. For the proposed structure the gain coefficient was calculated showing the possibility of light emission.

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