Machine-Learning-Enhanced NEGF Solver of Interband Cascade Laser

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***Abstract*—NEGF simulation of the interband cascade laser is performed taking into account various scattering proceses. The Hartree potential, important for device operation, is calculated by solving the Poisson equation with an excess charge approach. Support vector machine technique is used to effectively improve the charge classification. Results are compared with other methods of classification, showing a significant improvement.**

Keywords—Interband Cascade Laser, Non-equilibrium Greens Function, Support Vector Machine, Machine-Learning

I. Introduction

An interband cascade laser (ICL), which utilizes a type-II quantum well active region, has gained significant and continuously growing interest as a source of coherent light in the mid-infrared (MIR) wavelength region [1]. It can be used in various applications such as: trace gas detection, industrial process control, medical diagnostics, and free-space communication. Additionally, an area where the tunable properties of ICLs can be utilized is tunable diode laser absorption spectroscopy [2]. High quantum efficiency of ICLs is achieved thanks to the broken-gap alignment and cascading scheme similar to that of intersubband quantum cascade lasers (QCLs). Furthermore, ICL design can reduce the Auger recombination through the band-structure engineering.

Understanding of the principles governing the operation of ICLs is currently at a significantly lower level compared to QCLs, which were developed earlier. Because of this, considerable research still remains to be done to continuously refine our understanding and fill the knowledge gaps concerning ICLs, enabling ongoing improvements to meet ever-growing application-driven demands. Current GaSb-based ICL simulations have focused on improving issues such as electron and hole density imbalances in active wells, [3] or strain in active core analysis [4], but it is challenging to find simulations concerning quantum transport in these devices; to our knowledge, the only such a simulation of ICL is that of Sato *et al.* [5].

In this work, we used a powerful simulation method that provides a complete analysis, including in-plane carrier dynamics with quantum correlations, known as the non-equilibrium Green's function (NEGF) formalism. Transport equations were solved together with the Poisson equation, in which an excess-charge approach (ECA) is employed to interpret the particle density. In the standard approach, electron (hole) in conduction (valence) band state is considered to contribute a negative (positive) unit charge. In our approach, we employ the support vector machine (SVM) technique to improve the classification of the particles, which - in ICL - do not necessarily follow their above rules.

II. Method

A. Hamiltonian

Our NEGF solver utilizes a four-band upper block of 8 k·p Hamiltonian after the axial approximation [6]. It includes the first conduction band, heavy and light hole bands, and the spin-orbit band. Material parameters were adopted from Vurgaftman *et al.*'s paper [7]. The ICL is modelled by discretizing the Hamiltonian in z direction using the finite difference method [8]. Carrier dynamics in plane of the layers is represented by the in-plane momentum vector k_t. Strain was included in the calculations according to Bir and Pikus [9]. To avoid spurious solutions, that can arise in calculations, the Burt-Foreman parameter correction was used [10].

B. Quantum transport

Green's functions are calculated by solving the Dyson-Keldysh equations self-consistently. Their basis have the structure imposed by the basis of the Hamiltonian. Simulation of an „open" device, connected to the homogeneous leads, is possible through appropriate self-energies [11]. The scatterings on acoustic phonons, polar-optical phonons, ionized impurities, and interface roughness are included. Thomas-Fermi formula for the screening length is used in self-energy calculations. The treatment of scattering processes preserves their nonlocal nature.

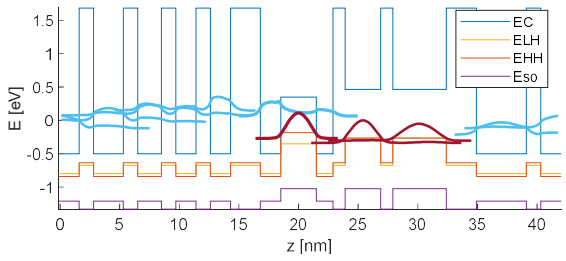

Figure 1. Carrier probability distribution in one period of ICL [3] simulated by 4 k·p solver. Colors indicate charge type based on the majority wave function component.

C. Poisson equation

Transport equations are calculated together with the Poisson equation with boundary conditions, which ensures neutrality of the ICL period [3], up to the point of self-compliance. It gets to some problems because in ICL, the distribution of majority/minority carriers can extend into minority/majority band. This is solved with a new charge classification method based on the SVM model. As training data, it uses carrier probability distributions calculated with

the Schrödinger equation using the same Hamiltonian as for the NEGF calculations. Training data depend on the shape of the probability function and the majority wave function component. Then, from the SVM method, a vector separating the two types of charges (delimiter) is calculated and used to determine free carrier densities from the lesser and greater Green's functions.

III. Results and Disscusion

Simulations are performed for one period of the ICL structure proposed by Vurgaftman *et al*. [3]. The bias voltage is chosen to satisfy the Bernard-Duraffourg condition [12], which is necessary for the photon emission. After each NEGF iteration, a new set of training data is calculated based on the potential obtained from the Poisson equation. Final results of this procedure are depicted in Figs. 2-3.

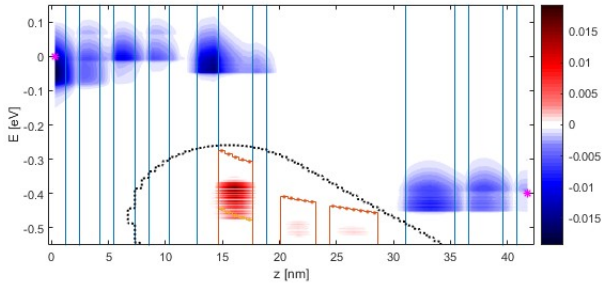

Figure 2. Density of electrons/holes calculated by NEGF simulator for one period of ICL [3] biased with the voltage 0.4 V/period. Fermi levels in the leads are indicated by pink markers on both sides of the device. Black dashed line depicts delimiter calculated using the SVM model.

In Fig. 2, the density of electrons/holes evaluated with the SVM-based method is shown with different (blue/red) colors. Charges appear to be properly classified: the electron (hole) injector is populated by the negative (positive) charge, as well as the upper (lower) energy level of the active region. In Fig. 3, charge densities obtained for two classification methods, the SVM-enhanced method and the standard method, are compared. Noticeable difference between these two methods is observed. In the electron injector area, due to the extension of carriers density into energy gap, a part of charge in omitted. The opposite effect is observed in the active region, where HH1 states extending into conduction band are treated as electrons. These problems result in the spurious peaks in charge density, like the ones marked with arrows, what makes the potential determined from the Poisson equation incorrect. Eventually, it can lead to difficulties in achieving the optical gain. On the other hand, the SVM-based method shows a solution without the spurious peak in charge densities and results in the positive gain enabling the emission of light.

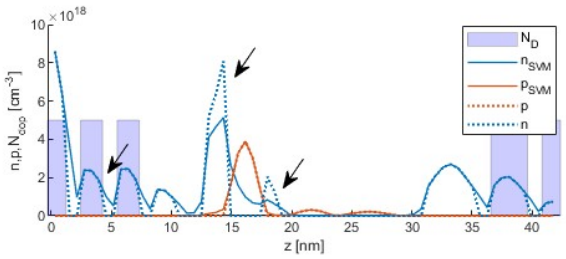

Figure 3. Doping and charge carriers (electrons/holes) density of one ICL period, calculated from the lesser/greater Green's functions. Calculations were performed for two classification methods: charges calculated with the standard/SVM-enhanced method are marked by the dotted/solid lines.

IV. Conclusion

In summary, we were the first to perform NEGF simulations of ICL in real space basis with various scattering mechanisms included in the formalism. We implemented the SVM method to improve the charge classification process, which otherwise could lead to the incorrect results in ICL simulations. The optimized simulation method shows good results comparable with other works [3]. Worth to note is that the method utilizing SVM does not cause any noticeable delays in calculations and could be implemented in the simulations of other quantum structures.

Acknowledgment

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