Numerical NEGF-based study of Urbach tails in III-V materials and superlattices

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***Abstract* — Numerical simulations that use the non-equilibrium Green's function (NEGF) method applied to an 8-band k·p Hamiltonian were performed for exemplary III-V material and superlattice with the intent to examine an influence of scattering processes on the formation of band tails. Results reveal that the Urbach parameter is not directly proportional to the value of perturbing potential but rather to its logarithm. It effects in a much modest temperature dependence of this parameter, which was reported in the literature for several III-V compounds. The values of the absorption coefficient estimated in the paper also remain in reasonable agreement with the experimental data reported in the literature for the bulk InAs and type-II InAs/InAsSb superlattice (SL).**

Keywords—Urbach tail, nonequilibrium Green's function, k·p Hamiltonian, InAs, InAs/InAsSb superlattice

I. Introduction

The studies of band tailing in semiconducting materials date back to the beginning of the 1960s [1]. Nevertheless, the agreement between existing theories and experimental data for III-V compounds is still not satisfactory [2]. For these materials, the actual band tail parameters are rather predicted from heuristic models that base on the parameters extracted from the experiments or results of numerical simulations [3]. The latter, apart from providing estimates of band tail parameters, can also add to better understanding of the phenomenon and its theoretical description. The knowledge about band tails enables resolving the difficulties in understanding of electronic and optical properties, such as reflectance, transmittance, and absorption-recombination coefficients in the subband gap region, which are important for the development of optical and photonic devices. Examples include, e.g., the existing consensus that excellent candidates for photovoltaic applications are materials with a band-tail width well below the thermal voltage [4]. On the opposite side are, e.g., Urbach-assisted electroabsorption-based modulators, in which tail states in the band gap can bring about strong electroabsorption and enable the effective realization of free-space optical communications [5].

In this paper, band tails in III-V materials are studied with NEGF formalism implemented in the full nondiagonal form, which distinguishes this work from previous NEGF-based studies [3]. It is important because the main mechanisms that build up the band tails, namely the scatterings on polar-optical phonons (POPs) and ionized impurities (IIs), are based on the long-range Coulomb interaction and thus are nonlocal.

II. Urbach Tail

The part of the density of states (DOS), which decays *exponentially* in the band gap region

$$N(E) \propto e^{-E/U_{c,v}}, \tag{1}$$

where energy E counts from the band edge into the gap, is known as the Urbach tail because of its direct connection with the Urbach edge of the absorption coefficient. The current understanding of the band tailing process is that it results from both static and dynamic disorders, which perturb the potential of an ideal crystal. It was argued that static and dynamic disorders are additive so that the Urbach parameter $U_{c,v}$ is the sum of the static and thermal components [6]

$$U_{c,v} = U(0) + U(T). \tag{2}$$

In III-V semiconductors, an electron interacts with the longitudinal optical (LO) phonons. This results in a temperature dependence of the Urbach parameter [7]

$$U(T) \propto \coth(\hbar\omega/2k_BT). \tag{3}$$

As for the static component, it was shown that (i) impurities influence the DOS not only due to the fluctuations in the dopants' concentration but also due to the scattering, (ii) most of the DOS "deformation" and gap shrinkage arise from the scattering effect, and (iii) the 'fluctuation' effect is important only at the energies far apart from the band edge [8]. The near-band-edge Urbach tail is then not affected by the topological disorder of the dopants. It can be well studied with a 'homogeneous' model, which includes the scatterings but ignores the randomness of the dopants' positions. This observation provides a justification for the current study.

III. Model and Method

The NEGF method is the one that can account for scatterings [3] and therefore is very appropriate to study the band tailing phenomenon. If applied in the full form to the multiband Hamiltonians, this method demands huge computational resources so additional approximations are necessary. The common procedure is to restrict the scatterings to the diagonal form enabling the use of efficient recursive algorithms [3]. However, both POP and II scatterings are, in principle, nonlocal so with this approximation some part of the physics is lost. In our approach, this restriction is dismissed: POP and II scatterings are considered in the full nonlocal form. The semiconductor is modeled with the 8-k·p Hamiltonian subjected to an axial transformation of the basis states [9]. It simplifies the calculations to a 4-band model. Essential for obtaining reasonable estimates is the consistency with the Poisson equation and the boundary conditions, which ensure charge neutrality. It is crucial because only then the chemical potential and the screening length, which both matter to the Urbach band, are set at the self-consistent values.

IV. Results

The study is limited to the exemplary bulk and superlattice (SL) materials, for which valuable experimental data are available from the literature, namely: the bulk InAs [10][11] and InAs/$InAs_{0.66}Sb_{0.34}$ SL [12]. Presentation of the results is further restricted to those in Figs. 1-3. Figure 1 depicts our

major finding: the significant difference between the theoretical line of Eq. (3) and numerical simulations. However, as can be seen, the latter is well-fitted with the equations:

$$U_{v,p-type} \cong \frac{-\hbar\omega}{B_v+\ln(l_{scr}[n_B+1+f(0)])}, \quad (4)$$

$$U_{c,p-type} \cong \frac{-\hbar\omega}{B_c+\ln(l_{scr}n_B)}, \quad (5)$$

where $\hbar\omega$ and n_B denote the LO-phonon energy and phonon population, $f(0)$ is the value of the Fermi factor at the band edge, l_{scr} is the screening length and $B_{v,c}$ are the temperature-independent coefficients. Equations (4) and (5) (as well as their equivalents for the n-type materials) can be derived by analyzing the scattering processes in the first Born approximation and will be provided in the future paper. Worth to note is that the disagreement of the simulation data with Eq. (3), observed in Fig. 1, is consistent with earlier experimental findings for various III-V compounds [2], including InAs [10] [11]. Then, our results can provide a reasonable explanation for these experiments. In the case of InAs, it is demonstrated in Fig. 2, which compares the simulations with the experimental data for the bulk n-type InAs, that a good agreement is found both above and below the absorption edge. Data in Fig. 3 demonstrate the capability of our NEGF solver for the reasonable prediction of the absorption coefficient, including the Urbach tail in the novel type-II SL materials.

V. Conclusion

The results presented in this work exhibit differences with theoretical models but simultaneously reveal good consistency with the experimental data available in the literature. They are not merely related to the performance of III-V devices but also to the more general issues connected to band tails. As an outcome from the analysis of numerical data, new analytical formulas for the Urbach parameter in III-V materials and devices were proposed. The capabilities of our NEGF solver to estimate the characteristics of the novel optoelectronic quantum structures and materials are also demonstrated.

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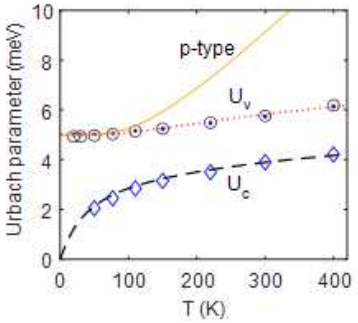

Fig. 1. Urbach parameter vs. temperature calculated for bulk InAs doped p-type to 10^{19} cm^{-3} (symbols) compared to the theoretical lines of Eq. (3) (solid-yellow), Eq. (4) (dotted-red) and Eq. (5) (dashed-black).

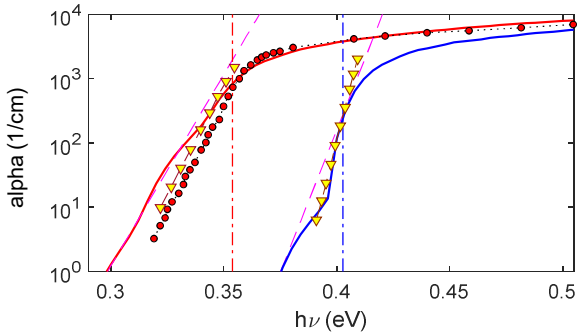

Fig. 2. Absorption coefficient calculated with the NEGF method for bulk n-InAs doped to 1.6×10^{16} cm^{-3} (solid lines) at 300 K (red) or 100 K (blue). Lines with symbols depict the experimental data of Dixon and Ellis [10] (circles) and Zotova *et al.* [11] (triangles). Dashed vertical lines indicate the position of the absorption edge. Dashed inclined lines have the slopes: U_{abs} = 7.3 meV or 4.9 meV calculated from the Urbach parameters $U_{c,v}$.

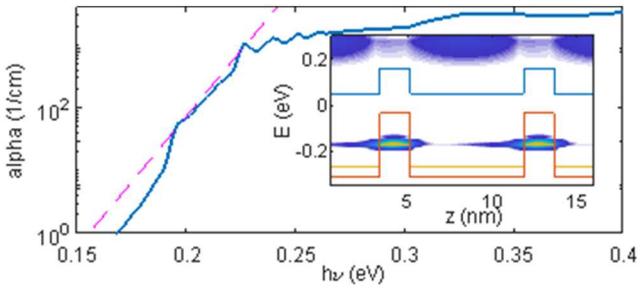

Fig. 3. Absorption coefficient calculated with the NEGF method for the strained InAs (6.7 nm)/$InAs_{0.66}Sb_{0.34}$ (1.8 nm) type-II SL at 240 K. Dashed line has the slope of 10.4 meV in the agreement with the experiment [12]. Inset: position-resolved density of states and SL bands profiles.

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