NEGF computation of optical absorption in InAs/GaSb type-II superlattices

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ABSTRACT

Optical properties of type-II broken gap semiconducting superlattice absorber are modelled within *interface layer approach*, using 8 band k·p Hamiltonian and nonequlibrium Greens function method. Good agreement with experiments over a wide range of temperatures for several structures is obtained for a common set of parameters, without the need for any adjustment. The studies cover the influence of scattering processes on absorption coefficient and miniband structure.

INTRODUCTION

In recent years, devices based on superlattice (SL) materials have attracted increasing attention. This is particularly true for the optoelectronics sector, which offers devices such as SL photo-detectors and quantum or interband cascade lasers. Due to their sophisticated architecture, complex band structure with nonparabolic dispersions, and technology-related features designing of such devices demands the use of numerical methods. Among them, the non-equilibrium Greens function (NEGF) method is one of the most advanced, since it is a fully quantum method. In the case of type-II SL (T2SL) absorbers, this method has been used to a very limited extent, mostly for studying the electronic transport [1][2]. In this paper the NEGF method is used for studying optical properties of T2SL InAs/GaSb absorbers. Results of numerical computations are compared with experiments showing good agreement. The benefits of the NEGF approach presented in the paper include, but are not limited to, studies of scattering-related features of the absorption coefficient and miniband tailing.

METHOD AND MODEL

The ingredient materials are modeled with the 8-band k·p Hamiltonian axially transformed to form two 4×4 uncoupled blocks [3]. Computations were performed separately for either of these blocks preserving the momentum representation for SL layers and the real space basis for the growth direction, z. The strain arising in SL structure was treated according to model solid theory [4]. All parameters were adopted from Vurgaftman's paper [5]. The size of simulated system was chosen to extend over two SL periods. The remaining part was accounted for through the boundary self-energies Σ_B which mimic the SL structure on both sides of the device. For this purpose the procedure of Ref. [6] formulated for multi-atomic layers of tight-binding Hamiltonians was adapted to SL case. The representative image of the simulated structure is depicted in Fig. 1. Results of the simulations are presented in Figs 2-6.

ACKNOWLEDGMENT

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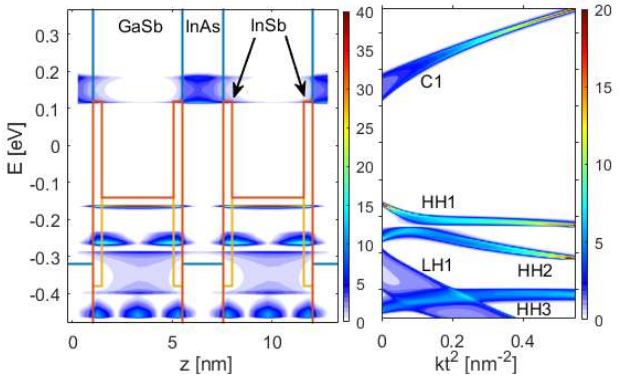

Fig. 1. Band diagram and position-resolved 1D density of states (left) and spatially averaged 1D density of states as a function of k^2 (right) calculated with the NEGF method for InAs/GaSb 25 Å/40 Å T2SL at 77 K. The arrows point at InSb layers, which are formed in SL with non-common-atom interfaces.

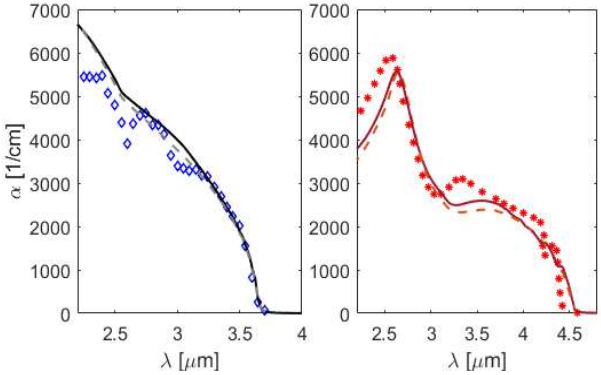

Fig. 2. Comparison between measured (symbols) and calculated (lines) absorption coefficient at 77 K for mid-wavelength infrared T2SL absorbers from Ref. [8] (left) and Ref. [7] (right). Calculations were performed using the NEGF method which includes (i) interface roughness scattering (IR) (dashed lines) and (ii) additional polar optical phonon scattering (solid lines). The main features of the absorption spectrum, its shape and magnitude as well as the cutoff wavelength agree very well.

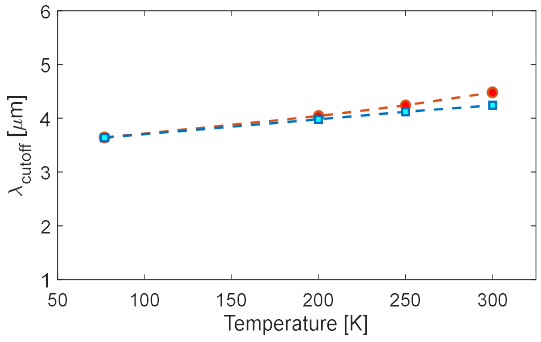

Fig. 3. Comparison between the cutoff wavelength of the absorption coefficient calculated using the NEGF method (circles) and experimental data [8] (squares) for an InAs/GaSb 18 Å/22 Å T2SL. Simulations for different temperatures were performed using identical set of parameters except of the lattice constant and the bandgap energy, for which the Varshni relation was used [5].

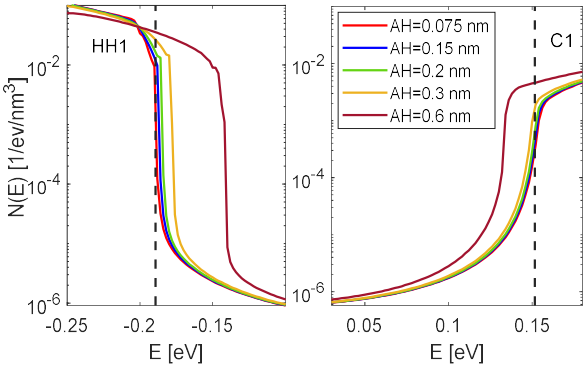

Fig. 4. Density of states calculated for an InAs/GaSb 18 Å/22 Å T2SL at 77 K. Dashed lines indicate edge of the C1 and HH1 minibands. Calculations were performed for different wales of asperity height (AH) of the interface roughness scattering included in NEGF method. With AH increasing, the bandgap narrowing (BGN) effect can be observed. In bulk materials such effect results from impurity scattering. The impact of IR-induced BGN on the absorption edge is shown in Fig. 5.

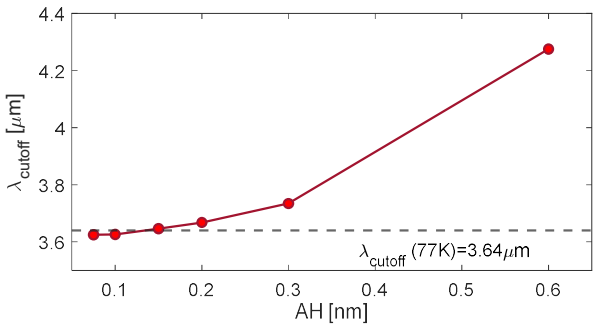

Fig. 5. The cutoff wavelength of the absorption coefficient calculated at 77 K using the NEGF method with interface roughness scattering for different values of asperity height (AH). The dashed line indicates the position of the absorption edge in experimental data [8].

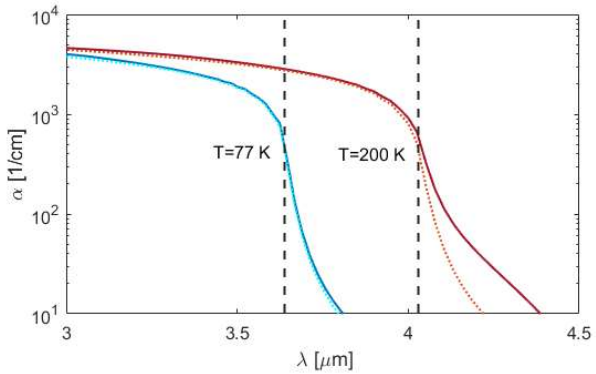

Fig. 6. Absorption coefficient calculated for an InAs/GaSb 18 Å/22 Å SL at 77 K (blue) and 200 K (red). Dotted lines represent data calculated with IR scattering, while solid lines represent data calculated with both IR and polar optical phonon scattering. Dashed vertical lines indicate the cutoff wavelength. The phonon contribution to the Urbach tail can be recognized at 200 K plot.