Silicon-Integrated Red-Light Optical Gain Medium Based on BGaAs/GaP Quantum Wells

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***Abstract*—In this study we present BGaAs/GaP quantum well (QW) structures integrated with GaP/Si virtual substrate as a promising structures for applications requiring red-light optical gain media. Gain spectra are computed based on an 8-band $k \cdot p$ model with an envelope function approximation and Fermi's Golden Rule. An emission of red light of wavelengths from the range of 730-690 nm is predicted for the QWs with 10-35% BAs mole fraction and widths below the critical thickness.**

I. Introduction

Light-emitting and lasing devices grown on Si wafers are topics of great interest among research groups focused on silicon technology. The devices can potentially allow to produce new Si-based optoelectronic circuits consisting integrated light sources and many approaches of manufacturing them are already researched. One of most recent is growth of GeSn alloys directly on the Si substrates [1]. Methods based on silicon itself consist of Er doping of Si, stimulated Raman scattering, and Si nanoparticles [2]. Also III-V semiconductor alloys, that are already widely used in the light emitting applications, can be grown by heteroepitaxy on Si to synthetize quantum dots, nanopillars or nanoneedles. Heterostructures made of III-V semiconductors can be attached to an amorphous Si layer in postprocessing to form a hybrid structure [3]–[5]. It is evident that the topic of the Si-integrated light emitters is already extensively researched but there still seems to be another new approach available.

Recent advances in growth technology allow to produce new materials containing boron atoms, such as BGaAs, BGaP, BGaAsP, BGaInP, BGaInAs, BGaAsBi, BAsBi, on GaAs, Si and GaP substrates [6]–[9]. The choice of BGaAs alloy for the QWs with barriers made of GaP allows a modelling of a simple novel system that may be systematically extended to more complicated cases in further theoretical works.

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II. Methods

A. Gain Modeling

Band-structures of bulk crystals are computed within the 8-band $\mathbf{k} \cdot \mathbf{p}$ model for zincblende crystals. Strain in the thin layer is homogeneous and included via the Bir-Pikus Hamiltonian. To calculate the band-structures of QWs, the above model is used including the envelope-function approximation expanded in a basis of planewaves. Local density of states function of free carriers and confined states are computed and used to calculate the quasi-Fermi levels of conduction and valence bands. For each simulation, 2-dimensional carrier concentration is defined for whole period of the structure. Schrödinger and Poisson equations are solved self-consistently with use of a predictor-corrector based method. The spectra are calculated according to Fermi's Golden Rule.

B. Material Parameters

GaP and GaAs are already well known compounds for which parameters are easily accessible in review publications or handbooks about semiconductors [10], [11]. On the other hand, BGaAs alloys are still under development. Some of their material parameters are yet not available (N.A.), well established or the calculations available require further experimental confirmation [12]. Despite of the lack of the some remaining parameters, we conducted our simulations approximating them to ones of GaAs. The choice is justified as the calculations concern lower BAs fractions in BGaAs alloys and are regarded as the preliminary predictions for the QWs.

III. Results and Discussion

A. Basic Characterisation of the System

A scheme of modelled single QW that is formed by the B_xGa_{1-x} as the thin layer surrounded by the strain free GaP barrier is shown in the inset of Fig. 1. The system is characterized by type I band offset forming more than 0.5 eV deep quantum confinement for both holes and electrons. However, indirect nature of GaP crystal weakens the confining effect of electrons in the system.

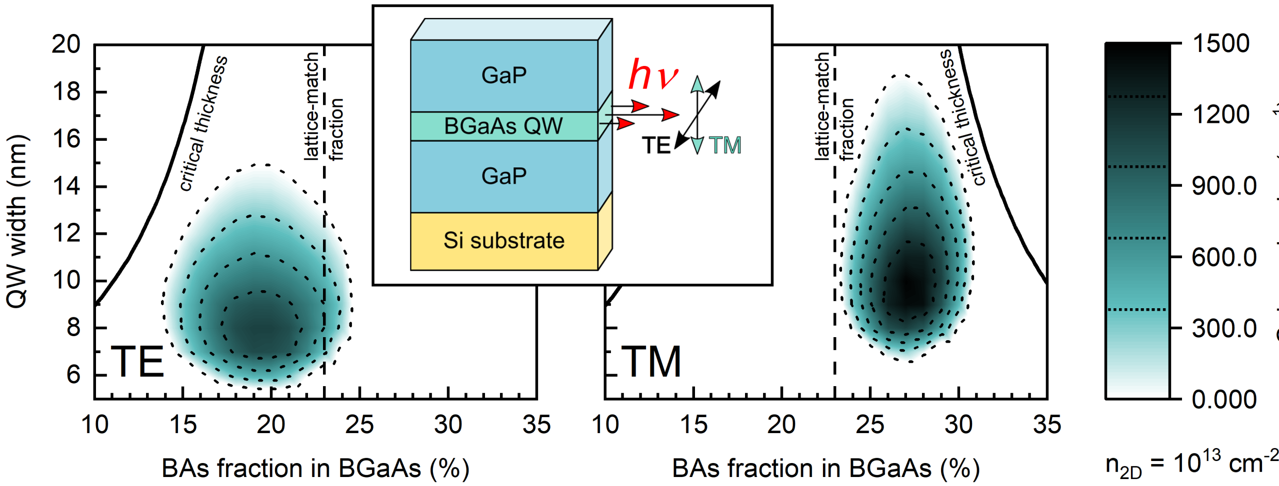

Fig. 1. Peak gain of quantum wells at room temperature in function of the QWs width and BAs mole fraction, schematics of the epitaxial structure consisting a single GaP/B_xGa_{1-x}As/GaP quantum well.

The most crucial for the system are conduction band minima dependencies on the BAs mole fraction in B_xGa_{1-x}. The significant Δ valleys splitting occurs since the structure is modeled to be grown on the (100) plane of GaP, and as a result, it defines the most advantageous BAs mole fraction range spanning from 10 to 35%.

B. BGaAs/GaP Quantum Wells

An analysis concerns a set of chosen representative strained and strain-free QWs. It begins with a presentation of main features connected to the carrier confinement and the QW positive charging effect and is followed by characteristics of gain spectra with their dependence on two-dimension carrier concentration n_{2D}. Next, an attention is focused on analyzing of the gain spectra and the peak gain for all representative QWs. Finally the topic is concluded with the peak gain maps for TE and TM polarization in function of the BAs fraction and the QWs width.

The importance of valleys in generating electric field around the QWs is highlighted. Carrier concentrations that are necessary to obtain positive values of the gain depends noticeably on the BAs fractions in BGaAs. Therefore, the fraction visibly affects the threshold current. Optimal BAs fractions in QWs are predicted to range from 14% to 31% and optimal widths are likely to be under the critical thickness. Thus, it is shown that the positive material gain can be achieved in the BGaAs/GaP QWs within the reasonable thickness and BAs fraction ranges with expected red-light (730-690 nm) emission.

IV. Conclusions

This study concerns BGaAs/GaP QWs grown on the GaP/Si virtual substrates that are theoretically analyzed within the multiband kp method and proposed as a promising optical gain media for red-light emitters. This material system appeared to be very promising for Si-compatible photonic integrated circuits since positive optical gain is achieved with reasonable QWs parameters. This study is among pioneer works investigating BGaAs QWs and therefore we believe that the presented results are the first road map for the development of BGaAs/GaP QWs for laser applications.

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