

# Continuous-band heterostructures: new concept for development of low-loss distributed Bragg reflectors for optoelectronic devices

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We introduced a new class of heterostructures (HS) that have no discontinuities for one of the band edges and, therefore, called continuous-band heterostructures (CBHs). The promising properties of CBHs are discussed by considering their optical and electrical characteristics. Our estimations show that CBH-based DBRs provide extremely low series resistance in comparison with conventional DBRs even at low level of doping that can be uniform. Low level of doping leads to low absorption. The absence of composition grading and doping profiles can simplify growth process. Results for some CBHs lattice-matched to GaAs are compared with those for conventional GaAs/AlAs structures.

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Vertical structure of a semiconductor laser or amplifier resonator with DBRs has a set of advantages in comparison with edge-emitting constructions. But some disadvantages are presented; they are concerned with a fact that mirrors of vertical structures are usually current-carrying excepting structures with intra-cavity contact structures [1]. Peculiarity of DBR for devices with vertical geometry consists in use of semiconductors as quarter-wavelength layers. Semiconductors with different chemical composition form multilayer heterostructure with a number of heterojunctions, half of which is forward-biased and half is reverse-biased. Low-doped structures have high resistance that leads to considerable electrical losses (thermionic voltage drop, drift-diffusion voltage drop, recombination losses, and parasitic capacitance). High level of electrical losses increases threshold current and leads to unwanted heating. The degradation observes not only in active area but in DBRs too [2]. The task of electrical losses decrease can be solved in different ways: grading of the profile of a DBR<sup>3</sup>, selective doping [3,4] and delta-doping [5], using of the superlattice-DBRs [6]. Graded DBRs reduce resistance only partially; the problem of high resistance still exists. By selective doping, it is possible to remove high influence of the discontinuity on carrier transport. However, it requires quite high doping level ( $\sim 1 \times 10^{18} \text{cm}^{-3}$  -  $5 \times 10^{18} \text{cm}^{-3}$ ) that leads to the increase of optical losses due to free carriers absorption (FCA). Application of superlattices leads to losses reduction but to reduction of the refractive indices difference as well.

In this work, we theoretically found a new class of HS. They are lattice-matched and have no band edge discontinuity for one of the bands. Due to absence of band discontinuity in these HSs, we refer to them as to continuous-band heterostructures (CBHs). In contrast to conventional heterostructures, CBHs can be formed by

intrinsic semiconductors and do not require any doping to form flat band edge. The estimations of electrical and optical properties of such structures show their superiority for layered DBR-like constructions.

All heterojunctions are usually considered in classification of several types with the following band lineups: straddling, Fig. 1a; staggered, Fig. 1d; broken-gap, Fig. 1e [7]. All of these HS can be grown using III-V semiconductors and their alloys. Thus, structures that are intermediate for stated types basically may be grown. We found that new important properties can be provided by CBHs (Fig. 1 b,c), which are intermediate for structures with straddling and staggered band lineups.

It is possible to find analytically all possible pairs of III-V semiconductors and alloys that provide lattice matching and continuous-band heterojunction. To implement the solution, it is necessary to solve coupled equations:

$$a_I = a_{II}, \quad (1)$$

$$E_{c_I} = E_{c_{II}}, \quad (2)$$

$$\text{or } E_{v_I} = E_{v_{II}}, \quad (3)$$

where  $a_{I,II}$  are the lattice constants;  $E_{c_{I,II}}$  and  $E_{v_{I,II}}$  are the band edges for conduction and valence band respectively.

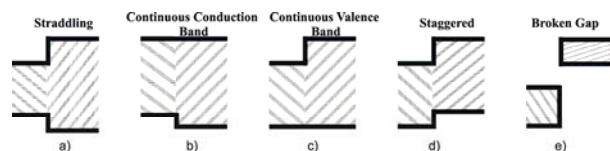


Fig. 1. Classification of heterojunctions.

We took parameters for binary III-V semiconductors from Refs. 8-10. The lattice constants are known to obey Vegard's law in (Al,Ga,In)-(P,As,Sb) ternary and quaternary alloys. Thus they are calculated by linear interpolation of binaries and band parameters are calculated taking into account bowing as in Ref. 10. Higher order interpolation formulas [11] can also be used. Anyway, if solutions are found in the linear approximation they will appear for higher order approximations with small corrections and final compositions should be verified experimentally.

As all parameters are constant for binary, functions of one variable for ternary and functions of two variables for quaternary compounds, Eqs.(1)-(3) can have point solutions for the heterojunctions binary-quaternary and ternary-ternary, and sets of solutions for the junctions ternary-quaternary and quaternary-quaternary and for the five- and six-component alloys as well. Application of the linear approximation and the affinity rule [12] to Eqs. (1)-(2) give us coupled algebraic equations which can be solved analytically. We solved them for heterojunctions  $A_x^{IIIorV} B_{1-x}^{IIIorV} C^{VorIII} / D_y^{III} E_{1-y}^{III} F^{VorIII}$ ,  $AB/C_x^{III} D_{(1-x)}^{III} E_y^V F_{(1-y)}^V$  and  $AB/C_x^{IIIorV} D_y^{IIIorV} E_{(1-x-y)}^{IIIorV} F^{VorIII}$ , based on Ga, Al, In, As, Sb, and P.

Fifteen solutions have been found, among them: GaAs/Ga<sub>0.54</sub>Al<sub>0.46</sub>Sb<sub>0.30</sub>P<sub>0.70</sub>, GaAs/In<sub>0.33</sub>Al<sub>0.67</sub>As<sub>0.79</sub>P<sub>0.21</sub>, InP/In<sub>0.39</sub>Ga<sub>0.61</sub>Sb<sub>0.14</sub>As<sub>0.86</sub>, GaSb/In<sub>0.41</sub>Al<sub>0.59</sub>Sb<sub>0.6</sub>As<sub>0.4</sub>, InP/In<sub>0.53</sub>Ga<sub>0.23</sub>Al<sub>0.24</sub>As and other.

Two coupled Eqs. (1)-(2) will have three variables for heterojunctions of kind  $A_x^{IIIorV} B_{1-x}^{IIIorV} C^{VorIII} / D_y^{III} E_{1-y}^{III} F_z^V G_{1-z}^V$  and  $A_x^{IIIorV} B_{1-x}^{IIIorV} C^{VorIII} / D_y^{III} E_z^{IIIorV} F_{1-y-z}^{IIIorV} G^{VorIII}$ . Let  $z$  be independent parameter with a range of values [0,1]. Lines  $x(z)$ ,  $y(z)$  will be the solutions in ranges  $0 \leq x(z)$ ,  $y(z) \leq 1$  for  $A_x^{IIIorV} B_{1-x}^{IIIorV} C^{VorIII} / D_y^{III} E_{1-y}^{III} F_z^V G_{1-z}^V$  and  $0 \leq x(z), y(z)$ ,  $1 - y(z) - z \leq 1$  for  $A_x^{IIIorV} B_{1-x}^{IIIorV} C^{VorIII} / D_y^{III} E_z^{IIIorV} F_{1-y-z}^{IIIorV} G^{VorIII}$ .

Eqs. (1)-(2) will have four variables for heterojunctions  $A_x^{III} B_{1-x}^{III} C_y^V D_{1-y}^V / E_z^{III} F_{1-z}^V G_m^V H_{1-m}^V$ ,  $A_x^{IIIorV} B_y^{IIIorV} C_{1-x-y}^{IIIorV} D^{VorIII} / E_z^{III} F_{1-z}^{III} G_m^V H_{1-m}^V$  and  $A_x^{IIIorV} B_y^{IIIorV} C_{1-x-y}^{IIIorV} D^{VorIII} / E_z^{IIIorV} F_m^{IIIorV} G_{1-z-m}^{IIIorV} H^{VorIII}$ . Let's take  $z$  and  $m$  as independent parameters with ranges of values [0,1], and find  $x(z, m)$  and  $y(z, m)$ . Range of  $z$  and  $m$  values, for which solutions satisfy to Eqs. (1)-(3), are defined by additional conditions:  $0 \leq x(z, m), y(z, m) \leq 1$  for  $A_x^{III} B_{1-x}^{III} C_y^V D_{1-y}^V / E_z^{III} F_{1-z}^{III} G_m^V H_{1-m}^V$  and  $0 \leq x(z, m)$ ,  $y(z, m)$ ,  $1 - x(z, m) - y(z, m) \leq 1$  for both  $A_x^{IIIorV} B_y^{IIIorV} C_{1-x-y}^{IIIorV} D^{VorIII} / E_z^{III} F_{1-z}^{III} G_m^V H_{1-m}^V$  and  $A_x^{IIIorV} B_y^{IIIorV} C_{1-x-y}^{IIIorV} D^{VorIII} / E_z^{IIIorV} F_m^{IIIorV} G_{1-z-m}^{IIIorV} H^{VorIII}$ .

Total list of pairs which provides non-point solutions consists of several tens of pairs for considered ternary/quaternary and quaternary/quaternary

heterojunctions based on (Ga, Al, In)-(As, Sb, P). Taking into account this number and the fact that each non-point solution is a continuous set of different compounds which have different properties, we can content that full set of solutions can provide perfect choice of required parameters (permittivities, lattice constants, carriers effective masses etc.) simultaneously with satisfying conditions (1)-(3).

Electrical properties of a HS are defined by its band diagram, doping and spatial carriers' distribution. For modelling of electrical properties of a DBR it is necessary to solve jointly continuity, drift-diffusion and Poisson's equations. But estimations can be obtained from simpler models. Band diagram for a single continuous-band heterojunction GaAs/Ga<sub>0.54</sub>Al<sub>0.46</sub>Sb<sub>0.30</sub>P<sub>0.70</sub>, defined in framework of affinity rule [12], is shown in Fig. 2.

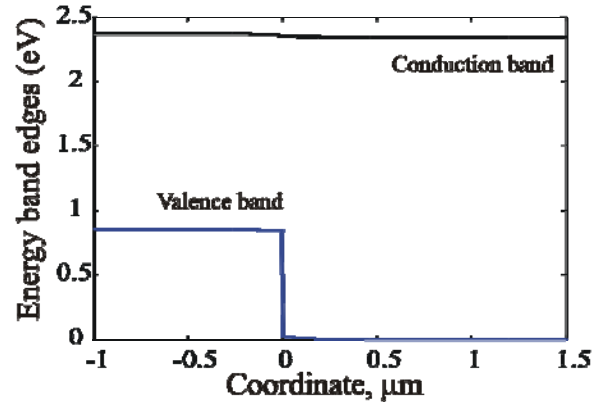


Fig. 2. GaAs/Ga<sub>0.54</sub>Al<sub>0.46</sub>Sb<sub>0.30</sub>P<sub>0.70</sub> continuous-band heterojunction.

As is seen from the figure, potential barrier in conduction band caused by difference of carriers effective masses and mobilities is small (Even for very high doping level it does not exceed 10 meV, that considerably less than temperature potential for room temperature. Valence band discontinuity is of about 820 meV. Flat conduction band edge provides low resistance of CBH both for forward and reverse bias. As a result, electrical losses in multilayer structures decrease. Thermionic voltage drop is the main source of electrical losses in DBRs<sup>5</sup>. Following<sup>5</sup>, at the absence of doping grading thermionic voltage drop for single GaAs/AlAs-heterojunction is of about 0.39 V for current density of 1000A/cm<sup>2</sup>. Estimations for GaAs/Ga<sub>0.54</sub>Al<sub>0.46</sub>Sb<sub>0.30</sub>P<sub>0.70</sub>-heterojunction give only 53 μV. So, this type of losses is almost excluded. The absence of the potential barrier also provides decrease of drift-diffusion voltage drop and capacitance resistance. It is expected that conductivity for carriers of one sign will be close to conductivity of bulk semiconductors.

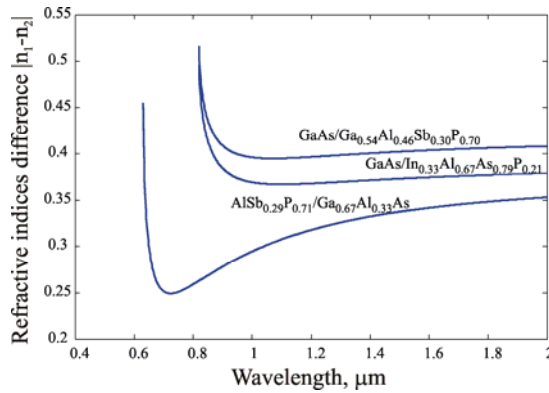


Fig. 3. Refractive indices difference for point solutions (Ga,Al)As-matched CBHs.

CBH can provide improvement of not only electrical but also optical properties of DBRs. For DBRs optical losses and refractive indices contrast has the primary importance. Optical losses are low for low-doped structures for energies less than band gap energy. Values refractive indices difference of point solutions lattice-matched to (Ga,Al)As-structures and GaAs/AlAs dependence on the wavelength are shown in Fig. 3. The calculations are implemented in framework of the model described in Ref. 10.

As is seen in Fig. 3, heterojunction GaAs/Ga<sub>0.54</sub>Al<sub>0.46</sub>Sb<sub>0.30</sub>P<sub>0.70</sub>, provides the highest refractive indices difference for selected point solutions. But this heteropair as well as GaAs/In<sub>0.33</sub>Al<sub>0.67</sub>As<sub>0.79</sub>P<sub>0.21</sub> does not allow to operate in short-wavelength optical range Pair AlSb<sub>0.29</sub>P<sub>0.71</sub>/Ga<sub>0.67</sub>Al<sub>0.33</sub>As can provide high indices contrast for wavelengths less than 0.7 μm.

Refractive indices differences of selected point solutions are less than for GaAs/AlAs (0.50-0.68 depending on wavelength). But GaAs/AlAs-pair has large band discontinuities, that leads to high electrical losses. Also, this pair can not be effectively applied for wavelengths less than 0.82 μm.

The most important parameters of DBR are the position of spectrum of refraction, refractivity in the maximum, and level of optical losses. Reflectance is determined by the refractive indices difference, number of pairs and losses level. Optical losses at the absence of interband transitions are determined by FCA. Following Ref. 13 FCA for a wide range of doping level can be approximated by linear dependence and for high concentration the dependence becomes parabolic. Selected CBH point solutions do not provide higher refractive indices difference than GaAs/AlAs. That is why DBRs based on this CBHs have lower reflectance and narrower stop-band at the same number of layers and doping level. But, estimations of the reflectance spectra taking into account FCA shows that CBH-DBR can provide higher

reflectance than GaAs/AlAs. Fig. 4 demonstrates reflectance spectra for low-doped CBH-DBR and high-doped GaAs/AlAs-DBR taking FCA into account. Both DBRs consist of 25 pairs. Lower refractive indices contrast for CBH-DBR provides narrower stop-band. But lower level of optical losses (Fig. 5) leads to the fact that this reflector has essentially higher reflectance in the maximum.

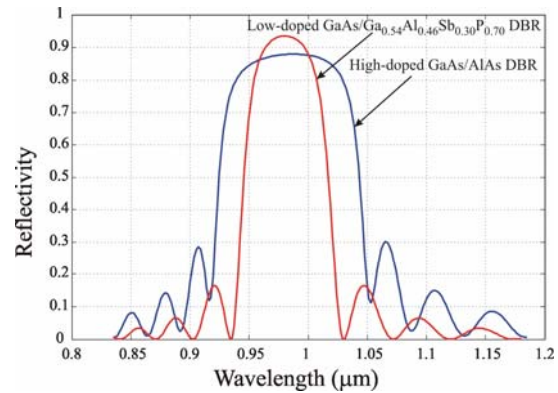


Fig. 4. Calculated reflection spectra for heavy-doped GaAs/AlAs- and low-doped CBH-DBRs, taking FCA into account.

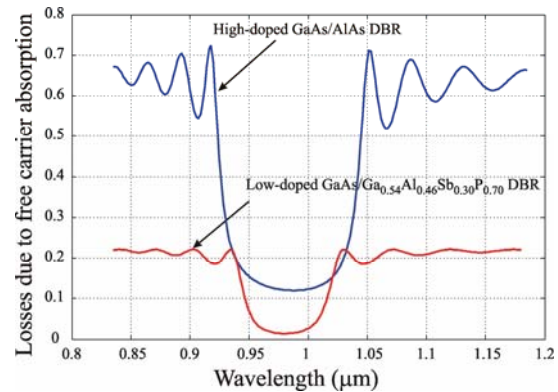


Fig. 5. Calculated of losses loss (1-R-T) spectra for heavy-doped GaAs/AlAs and low-doped CBH-DBRs.

Low level of electrical losses and optical absorption allows to increase number of layers without drastic increase of losses and obtain even higher advantages in comparison with high-doped GaAs/AlAs-DBR.

To conclude, we found, theoretically, new type of heterostructures – continuous-band heterostructures. CBHs having some properties usual for other HS provide unique properties concerned with particular carriers transport. It is expected that CBHs can find wide application for DBRs and band-engineering. Particular properties are expected for CBHs with high carriers effective mass contrast.

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