

Continuous-band heterostructures: a way for the development of low-loss distributed Bragg reflectors for optoelectronic devices

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It is introduced a new class of heterostructures (HSs), which have no discontinuities for one of the band edges and, therefore, can be named continuous-band heterostructures (CBHs). The promising properties of CBHs are discussed by consideration of their optical and electrical characteristics. Our estimations show that CBH-based DBRs provide extremely low series resistance in comparison to 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 the growth process. Results for some CBHs lattice-matched to GaAs are compared to those for conventional GaAs/AlAs structures.

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Vertically-emitting structures of semiconductor laser or amplifier resonators with DBRs have a set of advantages in comparison with edge-emitting constructions. But there are also some disadvantages present; they are concerned with the fact that mirrors of vertical structures are usually current-carrying excepting structures with intra-cavity contact structures [1]. DBRs for devices with vertical geometry consist in use of quarter-wavelength semiconductor layers. Semiconductors with different chemical composition form multilayer heterostructures 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 electrical losses increase the threshold current and lead to unwanted heating. The degradation observes not only in active area but in DBRs too [2]. The task of minimizing of electrical losses can be solved in different ways: grading of the profile of a DBR [3], selective doping [3,4], delta-doping [5] and the use of the superlattice-DBRs [6]. Graded DBRs reduce the resistance only partially (the problem of high resistance still exists). By selective doping, it is possible to remove the high influence of the discontinuity on carrier transport. However, it requires quite high doping levels ($\sim 1 \times 10^{18} \text{ cm}^{-3}$ - $5 \times 10^{18} \text{ cm}^{-3}$) that lead to the increase of optical losses due to free carrier absorption (FCA). Application of superlattices leads to losses reduction but to a reduction of the refractive indices difference as well.

In this work, we theoretically found a new class of heterostructures. They are lattice-matched and have no band edge discontinuity for one of bands. Due to absence

of band discontinuities in these heterostructures, 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 edges. The estimation of electrical and optical properties of such structures shows their superiority for layered DBR-like constructions.

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

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

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

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

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.

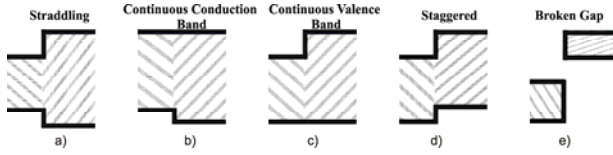


Fig. 1. Classification of heterojunctions.

We took the 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 the 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 the 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) gives coupled algebraic equations, which can be solved analytically. We solved them for heterojunctions $A_x^{IIIorV} B_{1-x}^{IIIorV} C^{VorIII} / D_y^{IIIorV} E_{1-y}^{III} F^{VorIII}$, $AB / C_x^{III} D_{(1-x)}^{III} E_y^V F_{(1-y)}^V$ 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_{0.54}Al_{0.46}Sb_{0.30}P_{0.70}, GaAs/In_{0.33}Al_{0.67}As_{0.79}P_{0.21}, InP/In_{0.39}Ga_{0.61}Sb_{0.14}As_{0.86}, GaSb/In_{0.41}Al_{0.59}Sb_{0.6}As_{0.4}, InP/In_{0.53}Ga_{0.23}Al_{0.24}As and others.

Two coupled Eqs. (1)-(2) will have three variables for heterojunctions of kind $A_x^{IIIorV} B_{1-x}^{IIIorV} C^{VorIII} / D_y^{IIIorV} E_{1-y}^{III} F_z^V G_{1-z}^V$ and $A_x^{IIIorV} B_{1-x}^{IIIorV} C^{VorIII} / D_y^{IIIorV} E_z^{IIIorV} F_{1-y-z}^{IIIorV} G^{VorIII}$. 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 $A_x^{IIIorV} B_{1-x}^{IIIorV} C^{VorIII} / D_y^{IIIorV} E_{1-y}^V F_z^V G_{1-z}^V$ and $0 \leq x(z)$, $y(z)$, $1 - y(z) - z \leq 1$ for $A_x^{IIIorV} B_{1-x}^{IIIorV} C^{VorIII} / D_y^{IIIorV} E_z^{IIIorV} F_{1-y-z}^{IIIorV} G^{VorIII}$.

Eqs. (1)-(2) will have four variables for heterojunctions $A_x^{III} B_{1-x}^{III} C_y^V D_{1-y}^V / E_z^{III} F_{1-z}^{III} G_m^V H_{1-m}^V$, $A_x^{IIIorV} B_y^{IIIorV} C_{1-x-y}^{IIIorV} D^{VorIII} / E_z^{III} F_{1-z}^{III} G_m^V H_{1-m}^V$ and $A_x^{IIIorV} B_y^{IIIorV} C_{1-x-y}^{IIIorV} D^{VorIII} / E_z^{IIIorV} F_m^{IIIorV} G_{1-z-m}^{IIIorV} H^{VorIII}$. By taking z and m as independent parameters with ranges of values [0,1], one can find $x(z,m)$ and $y(z,m)$. The 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 $A_x^{IIIorV} B_y^{IIIorV} C_{1-x-y}^{IIIorV} D^{VorIII} / E_z^{IIIorV} F_m^{IIIorV} G_{1-z-m}^{IIIorV} H^{VorIII}$.

The total list of pairs which provide 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 the full set of solutions can provide perfect choice of required parameters (permittivities, lattice constants, carriers effective masses etc.) simultaneously with the satisfaction of the conditions (1)-(3).

The electrical properties of a HS are defined by its band diagram, doping and spatial carriers' distribution. For the 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. The band diagram for a single continuous-band heterojunction GaAs/Ga_{0.54}Al_{0.46}Sb_{0.30}P_{0.70}, defined in framework of affinity rule [12], is shown in Fig. 2.

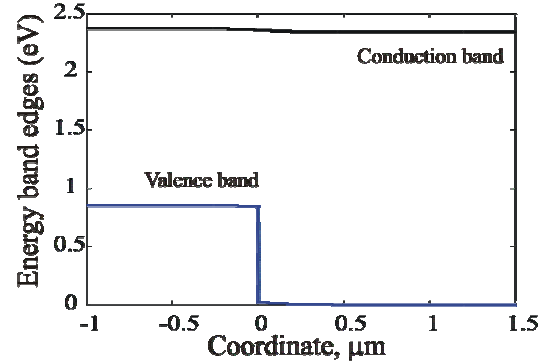


Fig. 2. GaAs/Ga_{0.54}Al_{0.46}Sb_{0.30}P_{0.70} continuous-band heterojunction.

As can be seen in the figure, the potential barrier in the conduction band caused by the difference of the carriers effective masses and mobilities is small (even for very high doping level it does not exceed 10 meV, that is considerably less than temperature potential for room temperature. The valence band discontinuity is about 820 meV. The flat conduction band edge provides low resistance of the CBH both for forward and reverse bias. As a result, the electrical losses in multilayer structures decrease. Thermionic voltage drop is the main source of electrical losses in DBRs. Therefore [5], at the absence of doping grading thermionic the voltage drop for a single GaAs/AlAs-heterojunction is of about 0.39 V for current density of 1000A/cm². Estimations for GaAs/Ga_{0.54}Al_{0.46}Sb_{0.30}P_{0.70}-heterojunction give only 53 μV. So, this type of losses is almost excluded. The absence of the potential barrier also provides a decrease of the drift-diffusion voltage drop and capacitance resistance.

It is expected that the conductivity for carriers of one sign will be close to the conductivity of bulk semiconductors.

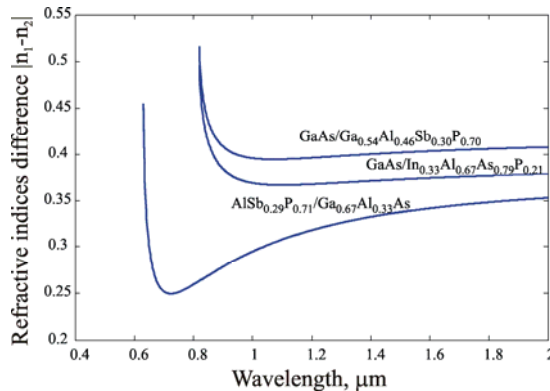


Fig. 3. Refractive indices difference for point solutions (Ga,Al)As-matched CBHs.

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

As is seen in Fig. 3, the heterojunction GaAs/Ga_{0.54}Al_{0.46}Sb_{0.30}P_{0.70}, provides the highest refractive indices difference for selected point solutions. But this heteropair as well as GaAs/In_{0.33}Al_{0.67}As_{0.79}P_{0.21} does not allow to operate in short-wavelength optical range Pair AlSb_{0.29}P_{0.71}/Ga_{0.67}Al_{0.33}As can provide high indices contrast for wavelengths less than 0.7 μm.

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

The most important parameters of DBRs are the position of the spectrum of reflection, the reflectivity 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 levels can be approximated by a linear dependence and for high concentration the dependence becomes parabolic. Selected CBH point solutions do not provide higher refractive indices difference than GaAs/AlAs. Hence 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 show that CBH-DBR can provide higher reflectance than GaAs/AlAs. Fig. 4 shows the reflectance spectra for

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

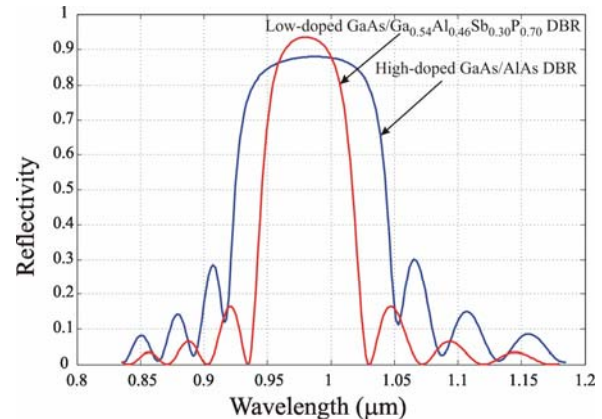


Fig. 4. Calculated reflection spectra for heavy-doped GaAs/AlAs- and low-doped CBH-DBRs, taking FCA into account.

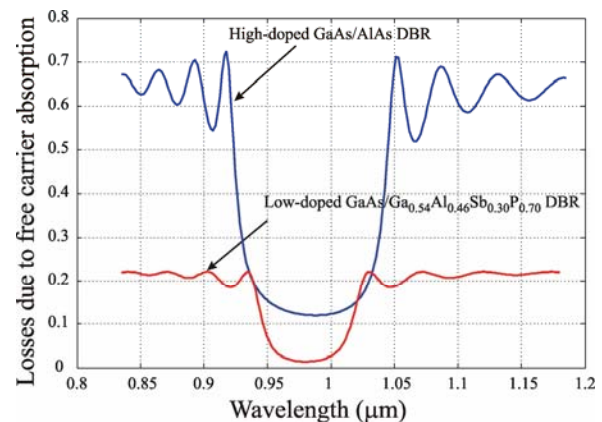


Fig. 5. Calculated loss (1-R-T) spectra for heavy-doped GaAs/AlAs and low-doped CBH-DBRs.

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

To conclude, we theoretically found a new type of heterostructures – continuous-band heterostructures. CBHs having some properties usual for other HSs 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 masses contrast.

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