Elimination of heterojunction band discontinuities by modulation doping

E. F. Schubert, L. W. Tu, G. J. Zydzik, R. F. Kopf, A. Benvenuti, and M. R. Pinto
AT&T Bell Laboratories, Murray Hill, New Jersey 07974

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Conduction- or valence-band discontinuities occurring at the junction of two heterogeneous semiconductors can be eliminated by appropriate doping of the interfacial region. We show by analytic and self-consistent calculations that simultaneous modulation doping and parabolic compositional grading result in flat band-edge potentials. The new concept is applied to distributed Bragg reflectors for vertical cavity lasers. The structures grown by molecular-beam epitaxy exhibit significantly lower resistances as compared to step-graded distributed Bragg reflectors.

Heterojunction band discontinuities have been an active field of research during the last decade[1] and made possible the realization of new device concepts such as modulation-doped transistors, heterobipolar transistors, and quantum-well lasers. The physical principles of these devices are based on heterojunction band discontinuities. In other device structures, however, heterojunction band discontinuities impede the flow of charge carriers across the junction. These structures include the optical distributed Bragg reflector which consists of alternating layers of two semiconductors with different refractive index, each having a thickness of a quarter wavelength. If distributed Bragg reflectors are used for current conduction, the constituent heterojunction band discontinuities impede the current flow, which is a highly undesired concomitant effect. It is the purpose of this publication to demonstrate that unipolar heterojunction band discontinuities can be eliminated by modulation doping and compositional grading of heterojunctions.

The charge carrier transport across a heterojunction is illustrated in Fig. 1, which shows the band diagram of two semiconductors "A" and "B." Band discontinuities occur in the conduction and valence band since the fundamental gap of semiconductor B is larger than the gap of A. Such discontinuities are usually referred to as type-I heterojunctions, which contrast to type-II (staggered) and type-III (broken gap) heterostructures. Transport across the heterojunction barrier can occur via thermal emission or via tunneling as schematically illustrated in Fig. 1. For sufficiently thick and high barriers, tunneling and thermal emission of carriers are not efficient transport mechanisms across the barrier. It is therefore desirable to eliminate such heterojunction band discontinuities in the conduction or valence band.

Modulation doping of a parabolically graded heterojunction will next be shown to result in a flat-band-edge potential. The band diagram of a parabolically graded conduction-band edge is shown in Fig. 2(a). The energy of the band edge increases parabolically with a positive second derivative between the points z_1 and z_2. The band edge further increases parabolically with a negative second derivative between z_2 and z_3. The energy of the band edge can be expressed as

$$E=\begin{cases} E_c(z_1)+\dfrac{\Delta E_c}{2(z_2-z_1)^2}(z-z_1)^2 & \text{for } z_1\leqslant z\leqslant z_2 \quad \text{(1a)} \\ E_c(z_1)+\Delta E_c-\dfrac{\Delta E_c}{2(z_3-z_2)^2}(z-z_3)^2 & \text{for } z_2\leqslant z\leqslant z_3. \quad \text{(1b)} \end{cases}$$

If the region $z_2\leqslant z\leqslant z_3$ is doped with donors of concentration N_D, electrons will transfer to the low-energy side of the junction, i.e., to the region $z_1\leqslant z\leqslant z_2$. In order to obtain a flat conduction band, the doping concentration, N_D, is selected in such a way that the depletion potential equals half of the heterojunction discontinuity, i.e.,

$$\tfrac{1}{2}\Delta E_c=(e^2/2\epsilon)N_D(z_3-z_2)^2. \quad (2)$$

For a given thickness of the graded region (z_3-z_2) and a given material system (ΔE_c), the equation allows one to determine the doping concentration which results in a flat band edge. That is, the depletion potential of the depleted donor layer exactly compensates for the built-in potential of the heterojunction.

Parabolic modulation-doped quantum wells were previously shown to result in a spatially *constant* electron concentration in the parabolically graded well.[2,3] The electron concentration adjusts itself in such a way that a flat-band edge results. The constant electron concentration has been demonstrated previously experimentally as well as by self-consistent quantum mechanical calculations.[2]

The calculated band diagram and the free-carrier concentration of a p-type GaAs/AlGaAs heterojunction are

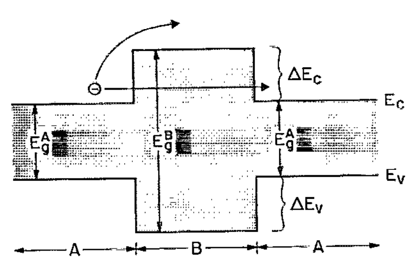

FIG. 1. Band diagram of a semiconductor heterostructure consisting of semiconductor A and B with band-gap energy E_g^A and E_g^B. Electron transport across the heterostructure can occur via thermal emission or via tunneling.

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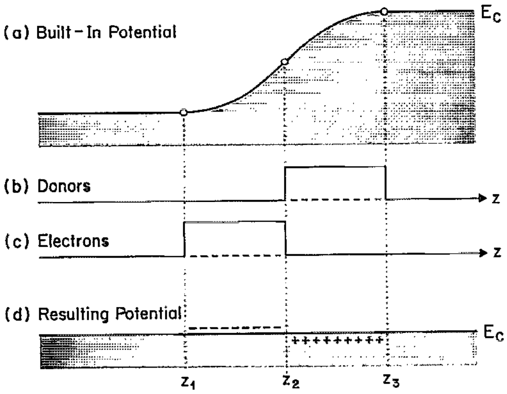

FIG. 2. (a) Parabolically graded interface of a heterojunction. The (b) donor profile and the resulting (c) electron distribution result in a (d) flat conduction-band edge due to compensation of the compositional built-in potential and the doping dipole potential.

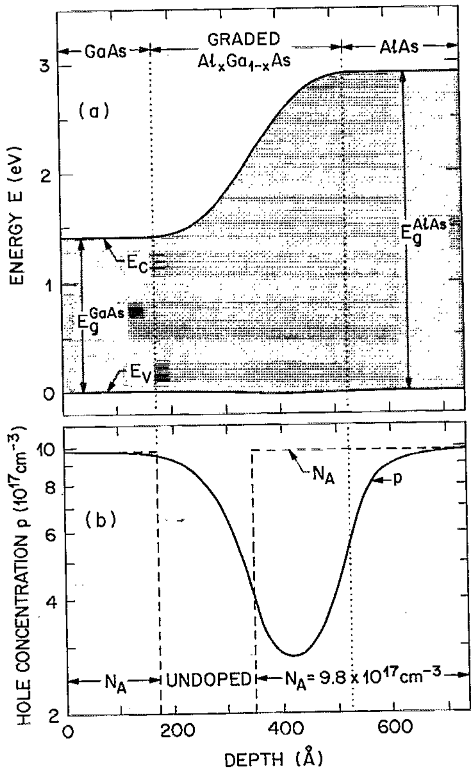

FIG. 3. (a) Calculated band diagram of a p-type modulation-doped, parabolically graded GaAs heterojunction. The entire band-gap discontinuity is confined to the conduction band. (b) Free-hole and acceptor distribution of the structure. Holes accumulate in the undoped region, while the doped region of the graded heterojunction is depleted of free carriers.

shown in Figs. 3(a) and 3(b), respectively. The self-consistent calculation, performed using a numerical partial differential equation solver,[4] demonstrates that the valence-band discontinuity is effectively eliminated. The free-hole and acceptor distribution demonstrate that (i) the graded doped region is depleted of free holes and that (ii) free carriers have transferred to the undoped part of the graded interfacial region. A residual modulation of the valence-band edge of 28 meV [Fig. 3(a)] is due to the spatial variation of the hole concentration in the depletion region. However, the residual modulation can be further reduced by increasing the doping concentration in the depleted region.

We finally note that band discontinuities can be eliminated in bipolar (p-n) heterojunctions by either homogeneous doping[5] or δ-doping.[6] Hayes *et al.*[5] used p-n doping combined with parabolic grading to minimize the base/emitter built-in voltage in heterobipolar transistors. We note, however, that the two concepts[5,6] cannot be applied to unipolar heterojunctions.

The concepts of elimination of band discontinuities is of importance for semiconductor devices with transport of carriers across unipolar heterojunction barriers, e.g., in distributed Bragg reflectors used in surface emitting lasers. The interfaces impede the current flow resulting in a large series resistance.[7–11] Several remarkable attempts were made to reduce the series resistance, including linear grading, step grading, and superlattice grading.[7–11] Note that the type and the shape of the grading do not alter the optical properties of the distributed Bragg reflectors significantly since only the fundamental Fourier component of the spatial varying refractive index determine the optical reflectivity.[12] Despite these efforts, the series resistance in surface emitting lasers still needs improvement. A laser-diode voltage drop <2 V is desirable, which has not yet been achieved in surface emitting lasers with GaAs/AlAs top and bottom distributed Bragg reflectors. Small diode voltages were achieved in surface-emitting laser structures with metallic mirrors,[13] indicating that the p-type multilayer reflectors are indeed the origin of the high series resistance of surface emitting lasers.

Distributed Bragg reflectors consisting of 20 quarter-wave pairs of p-type $AlAs/Al_{0.14}Ga_{0.86}As$ were grown on n^+-type (001)-oriented GaAs substrates by molecular-beam epitaxy. The interfacial regions of several samples were abrupt, step graded, and parabolically graded. The parabolically graded regions are modulation doped. The graded regions have total thickness of 350 Å and a doping concentration of $(1–5)\times10^{18}$ cm^{-3}. Optical reflectivity spectra of the reflectors yield excellent reflectivity ($>99\%$) centered at 850 nm.

The parabolic grading is achieved during molecular-beam epitaxial growth with a constant deposition rate of 0.3 μm/h by adjusting the Al- and Ga-effusion cell temperatures. The parabolic grading is evidenced by Auger electron spectroscopy. The Auger profile of a parabolically graded AlAs/GaAs reflector is shown in Fig. 4. The Al and Ga Auger electron signals exhibit parabolic transitions. No discontinuity or kink is evidenced for the Al and Ga signal in the transition region, indicating the suitability of continuous compositional grading to grow well-controlled profiles.

Current-voltage characteristics of a modulation-doped, parabolically graded structure and a step-graded structure are shown in Fig. 5. The differential series resistance of the mesa structure is evaluated at a current of 5 mA. Resistances of 98 and 185 Ω are evaluated for the modulation-

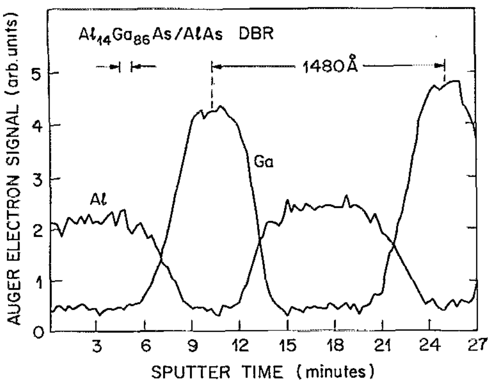

FIG. 4. Auger electron spectroscopy (AES) profile of a GaAs/AlAs multilayer structure with parabolically graded interfacial region. The profile is not corrected for different sputter rates in the AlAs and the GaAs.

doped, parabolically graded and the step-graded structure, respectively. The experimental results clearly demonstrate that the resistance of the modulation-doped parabolically graded structure is significantly improved. The contact resistance and the spreading resistance of the mesa structures are on the order of 2 Ω and do not continue significantly to the overall resistance ($R_{contact} = \rho_c / r^2\pi \cong 1.6$ Ω; $\rho_c \cong 5 \times 10^{-6}$ Ω cm^2; $R_{spreading} = \rho_{substrate}/4r \cong 0.5$ Ω;

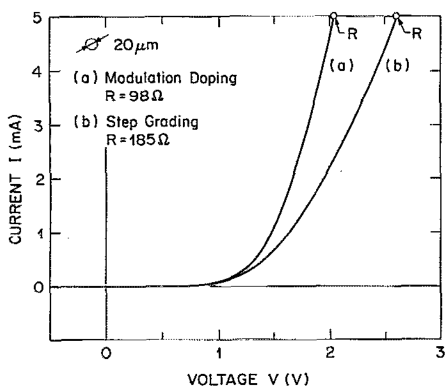

FIG. 5. Current-voltage characteristics of *p-n* junction diodes with 20-period *p*-type GaAs/AlAs distributed Bragg reflectors. The two characteristics are obtained from samples which employ (a) modulation doping and parabolic grading and (b) conventional single-step grading.

$\rho_{substrate} \cong 2 \times 10^{-3}$ Ω cm). Comparison of the measured resistance (304 $\mu\Omega$ cm^2) with the calculated resistance (16 $\mu\Omega$ cm^2) indicates a significant difference between the calculated and the measured resistance. The difference may be due to redistribution effects of Be in the AlAs. Recent experiments[14] indeed indicate that Be acceptors strongly redistribute in the AlAs even at relatively low growth temperatures.

In conclusion, we demonstrate for the first time that heterojunction band discontinuities can be eliminated in unipolar heterostructures by modulation-doped, parabolically graded heterointerfaces. The free-carrier/impurity dipole potential exactly compensates the compositional built-in potential. The elimination is evidenced by self-consistent potential calculations. Modulation-doped, parabolically graded AlGaAs/AlAs distributed Bragg reflectors growth by molecular-beam epitaxy have a significantly lower resistance as compared to conventional step-graded reflectors.

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