A NUMERICAL STUDY OF LATERAL P-N JUNCTIONS BETWEEN QUASI TWO-DIMENSIONAL ELECTRON AND HOLE SYSTEMS AT CORRUGATED GaAs/AlGaAs INTERFACES.

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Abstract

We report on our numerical method for modeling a novel lateral p-n-p quantum wire structure formed by surface orientation dependent Si-doping in corrugated *GaAs/AlGaAs* heterostructures. The two-dimensional conduction and valence band potential profiles are obtained for the electron and hole charge densities within a semi-classical Thomas-Fermi screening model. The non-linear Poisson equation is solved by Newton-Raphson iteration using the finite element method. Quantized electron and hole states at the heterointerface are subsequently obtained by solving the two-dimensional Schrödinger equation for the calculated potential profile. Sparse matrix finite element and subspace iterative techniques are used to calculate the lowest bound states of the system. We present the calculation results and discuss the advantages of fabricating quantum wires with this structure compared to conventional methods of electrostatic confinement.

I. Introduction

Recent experiments have demonstrated that Si behaves as a substrate-orientation-dependent amphoteric dopant in MBE grown *GaAs* and *AlGaAs*. Under suitable growth conditions, Si-dopants on {100} surfaces have donor behavior whereas Si-dopants on Ga-terminated {111}A surfaces have acceptor behavior [1-4]. These results have incited the investigation of lateral p-n junctions formed at selectively-etched and epitaxially regrown V-groove structures with exposed {111}A facets on normally exposed {100} substrates. Lateral *GaAs* p-n junctions with good diode I-V characteristics have been reported by Miller [3]. If Si-doped $Al_{0.3}Ga_{0.7}As$ is epitaxially grown on a semi-insulating corrugated *GaAs* substrate, then a lateral p-n junction may be realized between quasi two-dimensional electron and hole systems at the *GaAs/AlGaAs* interface. Ebner *et al.* [5] reported electroluminescence results which correspond to the *GaAs* quantum well band gap in such a system, and Harbury *et al.* [6] reported calculations which confirm the existence of a lateral p-n junction between two-dimensional electron and hole gas systems with Si-doping densities in excess of $5 \times 10^{17} cm^{-3}$.

We study a novel quantum wire design exploiting the amphoteric nature of Si in V-groove heterostructures resulting in lateral p-n-p junctions. V-groove structures have been previously explored for quantum wire designs, however this new design may offer some advantages compared to present unipolar structures [7] which use metal gate electrostatic confinement or side-wall etching. In section II we present our numerical method, section III contains the results of our calculations, and we conclude in section IV.

II. Methods

Figure 1 shows a schematic diagram of the model corrugated *GaAs/AlGaAs* heterojunction system. A 50 nm thick layer of Si-doped $Al_{0.3}Ga_{0.7}As$ is overgrown on an etched V-groove of a semi-insulating *GaAs* substrate. The side-walls of the V-groove expose the {111}A family of planes of the normally (100) terminated substrate. The chosen overlayer thickness and composition are similar to those of a lateral light emitting structure fabricated by Ebner *et al.* [5]. As indicated in Figure 1, the amphoteric Si-doped overlayer exhibits n-type behavior on the (100) surfaces and p-type behavior on the {111}A surfaces. The two-dimensional electron and hole gas (2DEG and 2DHG, respectively) shown in Fig. 1 forms along the heterointerface for suitable doping conditions.

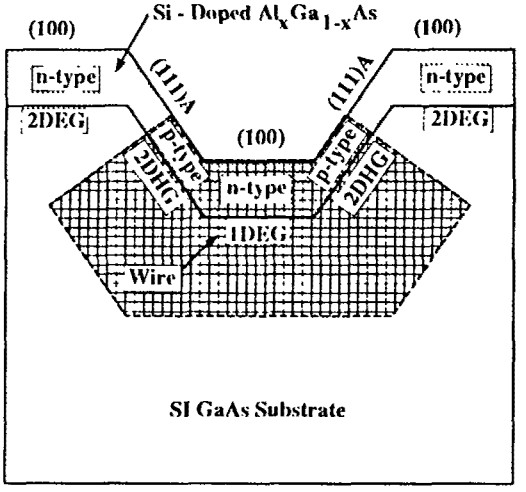

Figure 1: Schematic diagram of the model corrugated *GaAs/AlGaAs* heterojunction system.

The hatched region in Figure 1 represents the finite element calculation domain used to model the p-n-p quantum wire structure. The range of compositional mole fraction, doping type and density, and structural dimension are adjustable parameters of the system. A two-dimensional equilibrium potential profile of the model geometry is sought for different material parameters. The band bending of the electrostatic potential, $\phi(r)$, is obtained from the solution of Poisson's equation within a semi-classical Thomas-Fermi screening model.

$$\nabla^2\phi(r) = \frac{e}{\epsilon\epsilon_0}\left(n(r) - p(r) + N_A^- - N_D^+\right) \tag{1}$$

Complete ionization of the impurities is assumed at room temperature such that the background doping of the *GaAs* contributes to N_D^+ in the substrate, and the amphoteric Si-doping contributes to both N_A^- and N_D^+ in the overlayer region. The electron and hole densities, $n(r)$ and $p(r)$, respectively, are given by the Fermi-Dirac integral of order 1/2, $n(r) = N_c F_{1/2}(\eta)$ and $p(r) = N_v F_{1/2}(\eta)$, where η is the separation between the conduction or valence band edge and the electron or hole Fermi level, respectively. Space charge neutrality, at a point on the boundary deep inside the bulk substrate, fixes the electrostatic potential to the value which corresponds to a typical background doping of $1.0 \times 10^{15} cm^{-3}$. A Dirichlet essential boundary condition is used to pin the electrostatic potential deep inside the bulk. Natural Neumann boundary conditions are used on the remainder of the substrate boundary to model zero-field conditions. This provides a simple check on the converged result to confirm that charge neutrality conditions are satisfied at the boundary. An acceptable surface density of states along the (100) and (111) exposed facets is introduced by applying Dirichlet essential boundary conditions which pin the electrostatic potential on the surface to the near mid-gap value of 0.8 eV separation between the conduction band edge and the Fermi level. Invariance of the potential along the heterointerface, far from the p-n junctions, is modeled with natural Neumann boundary conditions at the left and right sides of the solution domain which force the potential to be flat along the boundary normal. The heterointerface discontinuity in the electrostatic potential is modeled as a linear constraint of the system along the interface.

The model domain is discretized with a highly non-uniform triangular mesh which preserves the angle between crystallographic directions. Large electrostatic potential variations occur over nanometer distances near the interface, surface, and p-n junctions, yet bulk space-charge neutral boundary conditions require the domain to extend on the order of microns into the bulk. A

highly non-uniform mesh is therefore essential in modeling realistic structures such as the p-n-p quantum wire. The node numbers are bandwidth optimized by a standard triangular element optimization algorithm. The Poisson equation is linearized by Newton-Raphson iteration and solved with finite elements and L/U decomposition. Linear constraints on the electrostatic potential at the heterointerface are implemented by the penalty method. The discretized Poisson domain consists of 16,168 elements and 8,427 bandwidth optimized nodes with a maximum element area of 1.2×10^4 Å^2 and a minimum element area of 70 Å^2. Convergence of the Newton-Raphson iterative procedure is obtained within twelve iterations at a typical cost of 430 cumulative seconds on an IBM RISC System/6000.

The confined states of the p-n-p quantum wire structure are also of interest. The wave-functions are sought by solving the two-dimensional Schrödinger equation for a previously computed potential profile.

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi(\vec{r}) + [V(\vec{r}) - e\phi(\vec{r})]\psi(\vec{r}) = E\psi(\vec{r}) \tag{2}$$

Here, $V(\vec{r})$ includes external potentials and band offsets and $\phi(\vec{r})$ is the electrostatic potential obtained from Poisson's equation. The quantum confined states satisfy either zero-valued Dirichlet or zero-valued Neumann boundary conditions which model the decay of the wave-function far from the electrostatic potential "pocket" which constitutes the quantum wire. Continuity of the wave-function across the heterointerface is modeled as a linear constraint. The resulting eigen-system is solved directly for the first few bound states with finite elements and subspace iteration. Linear constraints at the heterointerface are again implemented by the penalty method.

The model domain for the Schrödinger solution is a submesh of the Poisson domain containing the region of the electrostatic potential "pocket" at the tip of the V-groove. Bandwidth optimization and sparse matrix methods are employed in all the calculations for efficient storage and computation. The Schrödinger domain consists of 3,482 elements and 1,876 bandwidth optimized nodes. A converged solution of a 20 eigen-state subspace over 120 iterations typically consumes 240 cpu seconds on an IBM RISC System/6000.

III. Results

The following results for the quantum wire structure pertain to the calculation domain designated by the hatched region of the V-groove labeled 'Wire' in Fig. 1. Plotted in Figure 2 are the lateral conduction band minima and valence band maxima in the *GaAs* in a direction *parallel* to the heterointerface for an overlayer Si-dopant concentration of $1.0 \times 10^{18} cm^{-3}$ and a 100 nm n-region width. The center of the n-region is designated by zero distance and positions along the (111) and (100) are labeled at the top of the figure. Accumulation of electrons is expected in the region where the conduction band approaches and traverses the semi-classical Fermi energy indicated by the dashed line at 0.0 eV. The potential "pocket" is more clearly visible in the front and side views of the two-dimensional conduction band profiles shown respectively in the left and right insets to Fig. 2. The insets show only a portion of the full calculation domain which extends several microns into the bulk to ensure that bulk charge neutrality boundary conditions are maintained as discussed in Sec. II. It is expected that one-dimensional electronic states will be supported in the region labeled 'Quantum Wire' in Fig. 2.

The vertical conduction band profile, *perpendicular* to the (100), through the center of the n-region is plotted in Fig. 3 for the same doping and n-region width as in Fig. 2. The heterointerface is located at position zero; increasing negative values of distance correspond to positions deeper in the *GaAs* substrate whereas increasing positive values of distance correspond to the *AlGaAs* overlayer approaching the surface. The heterointerface "notch" is clearly visible in the *GaAs* where

the conduction band edge approaches and traverses the semi-classical Fermi energy designated by the dashed line at 0.0 eV. The two-dimensional ground state and first excited state of the quantum wire are shown in the left and right insets, respectively, of Fig. 3. The wave-functions are localized in the higher mobility *GaAs* at the heterointerface (the region of higher mesh density corresponds to the *AlGaAs* overlayer). Also shown in Figure 3 are the quantum wire energies for the first three states. The large ground state energy is attributed to the vertical heterointerface confinement whereas the nearly equal separations are attributed to the lateral p-n-p well confinement.

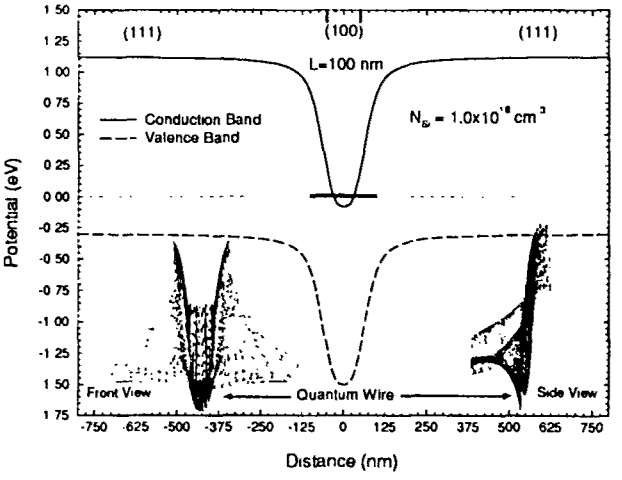

Figure 2: Lateral conduction band minimum *along* the heterointerface. The insets show the front and side views of the 2-D conduction band profile.

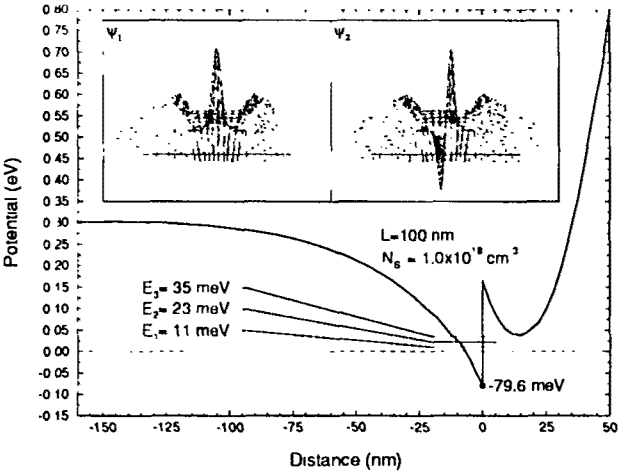

Figure 3: Vertical conduction band minimum *perpendicular* to the (100) at the n-region center. The insets show the ground and first excited states of the quantum wire.

IV. Summary

It is feasible to realize a quantum wire structure on a HEMT compatible corrugated *GaAs/AlGaAs* interface. These results indicate that the quantum wire level separations are controlled by the lateral confinement width. Such a structure has possible advantages compared to side-wall etched or Schottky contact electrostatically confined systems. The definition of the n-region width is controlled by the anisotropic etch time through an optically defined photoresist mask; ion-beam or electron-beam lithography is not required. This inherently bipolar structure might be used to inject minority carriers into the quantum wire from the p-regions, possibly leading to new device applications. If the p-type and n-type regions are separately contacted, by further nano-lithography, the lateral confinement width may be controlled by reverse biasing the p-n junctions and the electron Fermi energy might be controlled via a gate contact on the *AlGaAs*.

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