Type II broken-gap quantum wires and quantum dot arrays: A novel concept for self-doping semiconductor nanostructures

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A novel concept for creating self-doping quantum wires and quantum dot arrays based upon the InAs-GaSb material system is proposed. The unusual type II, broken-gap band line-up in this system allows charge transfer across the InAs-GaSb interfaces. We employ a recently developed coupled band formalism to examine analytically the band structure of InAs-GaSb quantum dots and wires. The analysis shows that appropriately engineered nanostructures which contain high free-carrier densities are possible without intentional impurity doping. Quantum dots in this system behave as artificial quasiatoms, with ionization energy and valence determined by fabricationally determined parameters. Synthetic *p-(n-)*type semiconductors may therefore be formed from arrays of InAs(GaSb) quantum dots embedded in GaSb(InAs). InAs-GaSb quantum wires are also investigated and found to exhibit self-doping behavior. Possible fabrication schemes utilizing recently developed technologies are discussed.

Progress in the field of nanostructure physics and fabrication has been motivated largely by the prospect of creating a new generation of electronic devices which rely upon quantum transport effects[1–3] for their operation. An issue that has not been adequately addressed is the question of how nanometer-scale transport structures might be doped. The stochastic nature of impurity dopant distributions is a critical problem in this field because the presence of an ionized impurity in the vicinity of a quantum wire or dot represents a significant electronic perturbation to these nanometer-scale structures. This discreteness also translates into uncertainty as to whether or not a given nanostructure in fact contains charge carriers.

In this letter we propose a novel class of nanometer-scale semiconductor structures for transport applications that avoids these problems. Employing a coupled band formalism recently developed for studying quantum wires and dots,[4–7] we examine analytically the band structure of quantum dots and wires based upon the type II system InAs-GaSb, and demonstrate the theoretical feasibility of creating self-doping quantum dot and quantum wire arrays which contain free charge carriers, without intentional impurity doping. This fact, along with the low effective mass of InAs which relaxes the size requirements necessary to observe quantum effects, make this new class of nanostructures potentially interesting for quantum transport studies. We conclude by examining the practical issue of how such type II quantum wires and dots might be fabricated.

The basic physics of InAs-GaSb heterostructures can be understood by reference to the inset of Fig. 1 , which shows the band line-ups of the system. Because the conduction-band edge of InAs lies below the valence-band edge of GaSb, charge transfer may occur across the interface.[8] Additionally, conduction-/valence-band mixing across the heterojunction is significant so that a multiple band model is necessary for theoretical calculations. A rigorous analysis should therefore be based on multiple band envelope function theory and should self-consistently include the band bending due to charge transfer at the InAs-GaSb interface (an example of such a calculation for superlattices is found in Ref. 9). Such an approach is quite computationally intensive, however. A flatband model is preferable because of its simplicity; and in spite of simplicity, the model successfully explains observations of a semiconductor-to-semimetal transition in InAs-GaSb superlattices.[10] This transition was observed to occur for InAs layer thickness in the neighborhood of 10 nm, in rough agreement with a Kane-type two-band calculation, which predicted a transition at 8.5 nm.[10] The approximate agreement of experiment with the flatband theory lends confidence that this simplified approach may be used as well to determine the essential characteristics of the type II quantum wire and quantum dot.

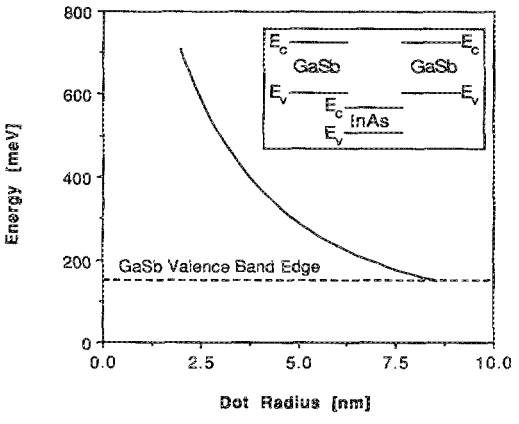

FIG. 1. Confinement energy of the lowest conduction-band state in a spherical InAs dot embedded in a GaSb barrier, plotted as a function of dot radius. The dashed line is the position of the GaAs valence-band edge, 150 meV above the conduction-band edge in bulk InAs. Inset: schematic drawing of the relative position of bulk InAs and GaSb conduction- and valence-band edges.

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Even in a flatband approximation, however, the study of the coupled band states in quantum wires and quantum dots is significantly more complicated than in the planar quantum well problem. The multidimensional nature of these heterostructures complicates the boundary conditions, and quantum wires or boxes of square cross section cannot be dealt with analytically since the finite square well potential is nonseparable in two or three dimensions. We therefore employ simpler geometries for which the heterostructure potentials are separable: a cylindrical quantum wire and a spherical quantum dot. A new envelope function theory has recently been developed which permits analytical solution of coupled band problems for these geometries.[4–7] The approach is based upon the observation that in a spherical band structure approximation such as the Kane model,[11,12] total angular momentum is a conserved quantity. Total angular momentum F is defined as the sum of the angular momenta J, of the zone-center Bloch functions and L of the envelope functions. In a cylindrical quantum wire the projection of total angular momentum along the wire axis therefore provides a good quantum number, F_z, while in a spherical quantum dot, the total angular momentum quantum numbers F and F_z are good quantum numbers. The Kane Hamiltonian may therefore be re-expressed in a basis of eigenstates of the operator F_z for the quantum wire, and in a basis of the eigenstates of F^2 and F_z for the quantum dot. Bulk eigenvectors in the new bases are then computed in the well and barrier regions just as in the familiar quantum well problem, and the requirement of continuity at the interface[13] results in an eigenvalue equation.

We illustrate the method by calculating the energy of the lowest conduction state in an InAs quantum dot embedded in GaSb (neglecting interfacial strain). The Kane Hamiltonian will be block diagonal with respect to quantum numbers F, F_z, and parity. Using the familiar rules of addition of angular momentum we form a total angular momentum basis as follows:

$$|k;F,F_z;J,L\rangle = \sum_{J_z=-J}^{J} \sum_{L_z=-L}^{L} \langle J,J_z;L,L_z|F,F_z\rangle \times |J,J_z\rangle\,|k;L,L_z\rangle\,. \tag{1}$$

The first term in the sum is the Clebsch–Gordan coefficient for adding states of angular momenta J and L. The states $|J,J_z\rangle$ are the band-edge Bloch functions, where $J=1/2$ for the conduction bands and $J=3/2$ for the upper valence bands.[11] The envelope kets $|k;L,L_z\rangle$ are free spherical waves with angular momentum quantum numbers L and L_z. These therefore have the coordinate representations

$$\langle\rho,\theta,\phi|\,k,L,L_z\rangle = \sqrt{(2/\pi)}\; i^L h_L(k\rho)\, Y_L^{L_z}(\theta,\phi)\,, \tag{2}$$

where h_L is a spherical Hankel function, $Y_L^{L_z}$ is a spherical harmonic, and k is the radial wave number.

Since states of different total angular momentum and total parity do not couple, each Hamiltonian subblock $H_{F,F_z\pi}$ may be separately diagonalized to obtain bulk eigenstates. We expect the lowest conduction state in a quantum dot to have even parity; this state turns out to have quantum number $F=1/2$, $F_z=\pm 1/2$. It is simple to show that for the conduction and upper valence-band system, the appropriate Hamiltonian subblock assumes the simple form[7]:

$$H_{1/2,\pm 1/2,\text{even}} = \begin{matrix} \\ |1/2,0\rangle \\ |3/2,1\rangle \end{matrix} \begin{matrix} \begin{matrix} |1/2,0\rangle & \quad |3/2,1\rangle \end{matrix} \\ \begin{pmatrix} E_c & -i\sqrt{(2/3)}\,pk \\ i\sqrt{(2/3)}pk & E_v \end{pmatrix} \end{matrix}, \tag{3}$$

where the quantum numbers k, F, F_z are understood in the basis vectors $|J,L\rangle$. In the matrix, p is the Kane matrix element.[11] E_c, E_v denote the conduction- and light-hole band edges. Diagonalization gives the familiar Kane two-band energy dispersion relations[12] inside and outside the dot:

$$(E_c^I - E)(E_v^I - E) = \tfrac{2}{3}|p|^2k^2$$

$$(E_c^O - E)(E_v^O - E) = -\tfrac{2}{3}|p|^2\lambda^2\,, \tag{4}$$

where superscripts I,O refer to regions inside and outside the dot, respectively. The exterior spherical wave number is taken as $i\lambda$ in anticipation of solving for bound energy eigenstates with energy $E > E_v^O$. Eigenvectors resulting from the diagonalization process have the form:

$$|\psi_E\rangle = A[\,|1/2,0\rangle + \sqrt{(E-E_c/E-E_v)}\,|3/2,1\rangle]\,, \tag{5}$$

where A is a constant to be determined by matching boundary conditions and applying normalization. The envelope parts of this vector are projected onto only the radial coordinate representation. This results in the following two-dimensional column vector:

$$\psi_E(r) = A\begin{pmatrix} h_0(kr) \\ \sqrt{(E-E_c/E-E_v)}\,h_1(kr) \end{pmatrix}. \tag{6}$$

The form of Eq. (4) is such that $\pm k(\pm\lambda)$ are degenerate roots. Using these roots and the basic form given by Eq. (6), state functions within each region are constructed. The requirement of regular behavior at the origin leads to combinations of Hankel functions within the quantum dot that are equivalent to spherical Bessel functions of the first kind. Outside the quantum dot, only the spherical Hankel function of imaginary argument which decays for large r is retained. Applying continuity of the resulting envelope states at the boundary of the quantum dot leads to the following condition:

$$\frac{j_0(kR)h_1(i\lambda R)}{j_1(kR)h_0(i\lambda R)} = \left(\frac{(E-E_c^I)(E-E_v^O)}{(E-E_v^I)(E-E_c^O)}\right)^{1/2}. \tag{7}$$

Equations (4)–(7) form a system of three equations in the three unknowns E, k, and λ.

The energy determined with this equation is plotted as a function of InAs dot radius in Fig. 1 using the material parameters of Ref. 8. We see that for dot diameters *larger* than 17 nm the lowest conduction state sinks below the position of the GaSb valence-band edge, implying that electrons transfer from the GaSb barrier into the InAs well region. In essence, the InAs quantum dot is behaving like

an artificial acceptor, in this case with a valence of 2. The ionization energy is determined by the position of the InAs conduction state with respect to the GaSb valence-band edge, a tailorable quantity dependent upon the radius of the InAs quantum dot. In similar fashion, a GaSb quantum dot embedded in InAs will behave as a donor. These observations suggest the possibility of creating a synthetic extrinsic semiconductor with one mobile carrier type (without intentional impurity doping) by fabricating two- or three-dimensional arrays of InAs(GaSb) quantum dots embedded in GaSb(InAs). Such a system would have an advantage over a conventionally doped semiconductor because individual quantum dots could be located precisely by lithographic means. We call attention to Ref. 2 where it is shown that appropriately tailored miniband structure in quantum dot arrays be used to suppress polar optical phonon scattering.

The InAs-GaSb quantum wire is studied in a manner similar to the quantum dot. The Kane Hamiltonian is expressed in a basis of eigenstates of the operator F_z in this case. Following a procedure similar to that taken for the quantum dot, we arrive at the eigenvalue equation for the lowest conduction state with $K_z=0$:

$$\frac{J_0(kR)H_1(i\lambda R)}{J_1(kR)H_0(i\lambda R)}=\left(\frac{(E-E_c^I(E-E_v^O)}{(E-E_v^I)(E-E_v^O)}\right)^{1/2}. \tag{8}$$

Using this equation, we find that for wire diameters greater than 13 nm, we expect charge transfer to occur across the InAs-GaSb interface. In this manner, quasi-one-dimensional channels may be created which contain high concentrations of free electrons, without intentional impurity doping. Due to the absence of charged impurity scattering centers, the quasi-one-dimensional nature of the electrons in the quantum wire, and the low effective mass of InAs we expect that such a structure would exhibit high mobility. Such a self-doping structure would be ideal for quantum transport experiments which require long scattering lengths.

A possible scheme for fabricating InAs-GaSb quantum wires and dots based upon a selective epitaxial growth process is shown in Fig. 2 . The process shown has recently been demonstrated in the GaAs-AlGaAs system resulting in passivated wire and dot structures with excellent morphology.[14] To apply the technique to InAs-GaSb, a thin masking layer of SiN would be deposited on a GaSb surface and selectively patterned by electron beam lithography to open holes and lines in the SiN layer. InAs is then grown selectively in the opening of the SiN layer. Finally the InAs is passivated by overgrowing GaSb. While effort would be required to develop such a selective epitaxy process in the

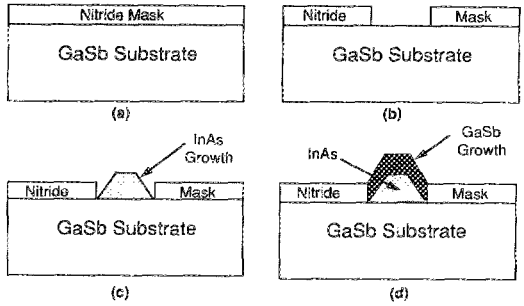

FIG. 2. Possible scheme for fabricating InAs quantum wires or dots embedded in GaSb using a selective epitaxial growth technique similar to that demonstrated for GaAs(AlGaAs) in Ref. 14. (a) SiN mask is deposited on a GaSb substrate. (b) Stripes or holes are created in the SiN mask by electron beam lithography followed by a chemical etch process. (c) InAs is grown selectively in the mask openings. (d) GaSb overlayer is grown epitaxially.

InAs-GaSb material system, the basic feasibility of the process has been demonstrated.

In conclusion, we have proposed a novel class of quantum wires and dots based upon the type II system InAs-GaSb, which is expected to exhibit unique self-doping behavior and high mobilities. This conclusion is based on a coupled band calculation which assumes a flatband condition. A more complete theoretical approach which incorporates band bending effects will be necessary to compute mobilities and carrier densities in such structures. Finally, we have suggested a scheme for fabricating such structures which could be realized by extending existing fabrication technology to the InAs-GaSb material system.

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