Infrared detector based on conduction band intersubband transitions in a heterojunction between two quantum wires.

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In this paper we study the feasibility of an infrared detector based on intersubband transitions in the conduction band of the junction between two semiconductor quantum wires. We show that by varying the radius of the wires it is possible to engineer a band structure of the junction that would be favorable for creating and detecting photocurrent. The suggested concept also allows for broadband detection based on arrays of wires with different radii.

Infrared (IR) photo detectors operating in the medium wavelength IR between 3-5 µm, long wavelength IR between 8-12 µm, and very long IR, are important for many applications including thermal imaging and remote sensing. Intersubband transitions are a typical mechanism for quantum well infrared photodetection, and have various attractive features. First, the position of the subbands depends significantly on the geometric dimensions of the system, and can be effectively controlled. Second, phonon scattering is reduced by the quantum confinement, enabling the detector to operate at higher temperatures. However, quantum well infrared photodetectors have one significant disadvantage: intersubband transitions in these systems cannot be excited by light at normal incidence. Therefore, one needs to use special coupling mechanisms such as two-dimensional grating couplers. One way to avoid this problem and simplify the design of the detectors is to replace quantum wells with quantum wires that do not suffer from this drawback.

Thus, using quantum wires instead of quantum wells, one can develop more convenient detectors sensitive to normally incident light. Using the nanopatterned template technique, one can fabricate quantum wires with a predefined radius and length. Aluminum is anodized in an electrochemical cell where it serves as the anode, while a platinum electrode serves as the cathode. The applied anodizing voltage primarily controls the diameter and spacing of the pores in the template. The diameter can be varied from a few nanometers to about 100 nanometers with a pore depth of a few microns. This technique, therefore, allows for applying band gap engineering to quantum wires. Using this technology, one can create a focal plane array of the detectors tuned to several wavelengths of IR radiation. One advantage of this template technique is that fabrication can occur on the final substrate, which can also support the electronic circuits necessary for the performance of the detectors.

In this paper we present initial calculations for a proposed mechanism for developing such detector arrays. The structure uses a heterojunction between two quantum wires (active and barrier layers). The active layer is n-doped, while the barrier layer is undoped. In the structure, the active layer terminates at a metallic contact and the barrier layer terminates at a transparent conducting oxide, which is exposed to the incident light. The quantum wires are grown in the template and, therefore, have the same diameter as the nanopatterned structure. The small size of the quantum wire results in the quantization of the conduction band energy levels.

The radii of the wires are selected in such a way that the band structure is similar to the one shown in Fig. 1. In the structure, the active layer terminates at a metallic contact and the barrier layer terminates at a transparent conducting oxide, which is exposed to the incident light. The ground state, $E_{1}^{a}$, of the active layer wire is slightly higher than the first excited state, $E_{2}^{a}$, of the active layer wire. In the absence of IR radiation, only the lowest subband, $E_{1}^{a}$, of the active layer is populated with electrons, which do not have sufficient energy to overcome the potential barrier across the junction. The absorption of IR energy moves some of the electrons from $E_{1}^{a}$ to the next higher subband $E_{2}^{a}$. In the presence of the bias, these higher energy electrons can easily cross into the barrier layer, thus producing a photocurrent. An accurate modeling of such a detector and calculation of its characteristics requires a self-consistent analysis of the carrier kinetics and the band structure of the system in the vicin-
ity of the junction. Before that, however, it is important to determine if the suggested concept is at all possible. In order to answer this question we investigate the conditions needed to produce a band diagram as shown in Fig. 1 by varying radii and chemical compositions of the active and barrier layers.

Thus, the main task of this paper is to calculate the structure of subbands in the conductive band of two possible candidates for these detectors, namely, CdS and CdSe. Since we are only interested in conduction subbands, we can solve a simple single-band problem for the conduction electron on the radius of the quantum wire for CdSe (dashed line) and CdS (solid line) for longitudinal wave number \( k_z \) equal to zero. Energy levels of CdS are shifted up 150 meV due to the conduction band discontinuity.

The energy levels of the confined electron are counted as a function of the radius of the quantum wire.\(^{13}\) Thus, the main task of this paper is to calculate the energy levels of the confined electron for \( \hat{H} = -\frac{\hbar^2}{2m_e} \Delta + V(\rho) \), where \( m_e \) is the effective mass of electron, and \( V(\rho) \) is defined as

\[
V(\rho) = \begin{cases} 
0 & \text{for } \rho \leq R, \\
\infty & \text{for } \rho > R.
\end{cases}
\]

Here \( R \) is the radius of the wire, which, we assume to have the shape of a cylinder. Using the cylindrical symmetry of the system and the homogeneity along \( z \), we can find solutions to the respective Schrödinger equation in the form

\[
\Psi_{n,m}(\rho, \phi, z, k_z) = A_{n,m}J_n(\kappa_{n,m} \rho)e^{im\phi}e^{ik_z z},
\]

where \( \kappa_{n,m} \) are the \( m \)-th zeroes of the \( n \)-th order Bessel function, \( J_n(\kappa_{n,m} R) = 0 \).

The boundary conditions at the infinite potential well require the wave function to vanish at the boundary. Thus the energy subbands are determined by zeroes of the Bessel function:

\[
E_{n,m}(k_z) = \frac{\hbar^2}{2m_e} (\kappa_{n,m}^2 + k_z^2).
\]

The energy levels of the confined electron are counted from the bottom of the conduction band. Fig. 2 shows the positions of the bottoms (\( k_z = 0 \)) of several lowest subbands for CdS (\( m_e = 0.21m_0 \), where \( m_0 \) is the mass of the free electron) and CdSe (\( m_e = 0.13m_0 \)) as a function of the wire radius. The energy in this figure is counted from the bottom of the conduction band of CdSe, which lies 150 meV below the conduction band of CdS. This figure shows that by choosing the radius of the wire, we can engineer energy subbands in the active and barrier wires in a configuration, optimal for detecting light of a particular frequency. As an example, we consider the CdSe/CdS system. For this detection scheme to work, the first excited subband in the active CdSe layer should lie above or at the lowest subband of the barrier CdS material. Fig. 2 shows that this condition may only be fulfilled if the radius of the wire is no larger than 41.7 Å. For the CdSe quantum wire of radius 40 Å the ground state energy \( E^{CdSe}_1 \) is equal to 106 meV and the first excited state energy \( E^{CdSe}_2 \) is equal to 270 meV. The lowest subband in CdS, in this case, lies slightly below \( E^{CdSe}_2 \) in CdSe. Thus, the structure with this radius can be used to detect IR photons with the wavelength 7.57 \( \mu m \).

Once the band structure is determined, we use the first-order perturbation theory to calculate absorption spectra of the single heterostructure:

\[
\alpha(\omega) \sim \frac{1}{m_\omega R^2} \sum_{f,i} \int dk_z \left| \left\langle f | \hat{H}_{rad} | i \right\rangle \right|^2 \times \delta(E_f - E_i - \hbar\omega)[F(E_i) - F(E_f)],
\]

where \( F \) is the Fermi-Dirac distribution function; \( f \) and \( i \) represent the set of quantum numbers specifying final and initial states of the electron. \( \hat{H}_{rad} \) here is the interaction Hamiltonian between the electron and electromagnetic field in the Coulomb gauge: \( \hat{H}_{rad} = \frac{e}{m_0} \mathbf{A} \cdot \mathbf{p} \), where \( \mathbf{A} \) is the vector potential of the electromagnetic field and \( \mathbf{p} = -i\hbar \nabla \) is the linear momentum operator. Evaluation of the matrix elements in Eq. 5 reveals the selection rule, \( n_f = n_i \pm 1 \), and the necessity for the incident radiation to be polarized perpendicularly to the axis of the wire. The momentum of the photon is assumed to be...
where we have introduced the conduction band of CdSe.

FIG. 3: (a) Absorption spectra of intersubband transitions in the conduction band of CdSe of radius 40 Å for temperature 300 K. In this figure, the positions and relative heights of different peaks at the same temperature reveal relative contributions of various transitions to the spectrum. In the case of CdSe we can see that, at all temperatures, only the transition from the lowest to the first excited subband contributes to the spectrum. Other transitions are strongly suppressed even at higher temperatures because of the small population of the respective subbands. It should be noted, however, that when calculating the spectra we introduced a small temperature independent broadening parameter in order to regularize the δ-function.

As another example we consider the CdS/CdTe heterojunction, the band alignment parameters for which can be found in Ref. 8. Analysis of the subband structure for this system shows that in this case there is an alternative way for transportation of the electron from the active wire to the barrier wire. At a radius equal to 74 Å, the first excited states in both semiconductors are almost degenerate. This allows for the electron excited by the 26.03 μm photon to the first excited subband in CdTe to move to CdS, occupying the first excited state in this material. For illustration, we also show in Fig. (3b) the absorption spectra of a CdTe wire (radius 104 Å) for temperatures of 100 K and 300 K. Unlike the case of CdSe, in this material increasing the temperature results in more transitions becoming visible; however, the main transition corresponding to the 51.69 μm photon still remains more intensive at all temperatures.

Our calculations show the feasibility of designing an IR detector based on intersubband transitions in the junction of two different semiconductor quantum wires with the same radii. Variations of the radii and conduction band offsets enables one to determine the optimal structure required for the detection of a single IR wavelength. Additionally, focal plane arrays of quantum wires incorporating different parameters can be used to detect a range of wavelengths.

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