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QUANTUM WELL WIDTH AS AN UNCERTAINTY SOURCE IN ELECTRONIC TRANSITIONS: A SIMULATED APPROACH

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Abstract – Semiconductor heterostructures of nanometric dimensions represent a challenge in Metrology, requiring innovations and new developments. A single quantum well is the simplest structure of this nature, the basis for many optoelectronic devices, like lasers. In this work it is calculated the eigenstates of electrons, light holes and heavy holes of quantum wells of GaAs into $Al_{0.2}Ga_{0.8}As$. It was varied the width of these wells by typical monolayer values, and evaluated implications in the electronic transitions from valence band to conduction band. Results demonstrated that uncertainties as less as 0.35 nm in the quantum well width cause optical transitions up to 13meV.

Keywords: quantum well, heterostructure, electronic transition.

1. INTRODUCTION

The use of devices based on quantum mechanics effects are growing. Semiconductor heterostructures of nanometric dimensions represent a challenge in Metrology, requiring innovations and new developments [1,2]. The single quantum well is the simplest structure of this kind, the basis for many electro optics devices, like lasers. It consists of a layer of a material of band gap smaller than the surrounding material, like in the figure 1.

For this quantum well structure, without doping, the band profile is shown in figure 2.

In the direction orthogonal to the GaAs plane (growth of epitaxial layers), the electronic behavior is quantized inside the well, for small widths of few angstroms. The localized eigenstates and eigenenergies inside the well could be calculated for electrons in the conduction band, CB, and for light (LH) and heavy (HH) holes in the valence band, VB.

The eigenstates are called sub-bands in the well.

The electronic transitions from sub-bands in the CB to the VB are very important results for optoelectronic applications.

These transitions could be evaluated by many techniques, like photoluminescence and photocurrent.

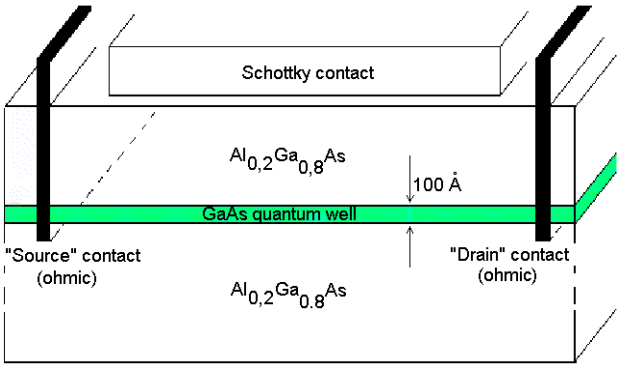

Fig. 1. Sketch of a semiconductor heterostructure of quantum well type. There is a 100 Å quantum well of GaAs inside $Al_{0,2}Ga_{0,8}As$. The contacts shown are typical for use in a MODFET (modulated doped field effect transistor).

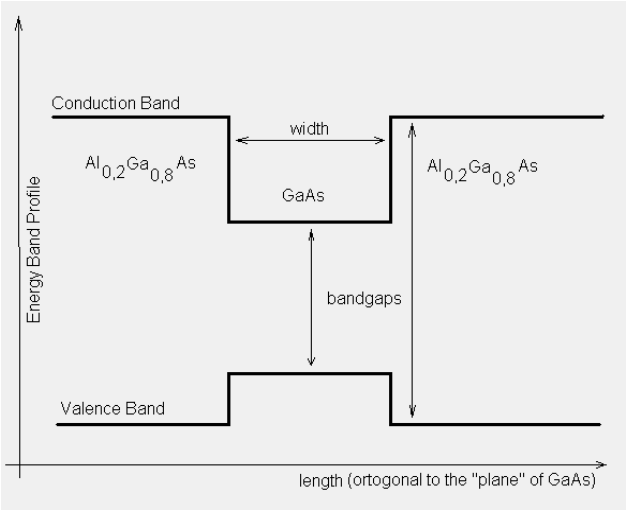

Fig. 2. Sketch of the band structure at a point of the direct band gap semiconductors.

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In this work a numerical model, based on a fully quantum-mechanical solution of Schrödinger equation, in an effective mass approach, was used to calculate the eigenstates of electrons, light holes and heavy holes of quantum wells of GaAs into $Al_{0.2}Ga_{0.8}As$ [3-7].

It was varied the width of these wells by typical monolayer values that could be a source of experimental uncertainty. The scope of this work is to evaluate some implications of this uncertainty in the electronic transitions.

2. MODEL DESCRIPTION

The model is based on the effective mass approximation, where the electron wave function is taken as the product of a Bloch function and an envelope function, solution of the time-independent Schrödinger equation:

$$H\phi_i = E_i\phi_i \qquad (1)$$

E_i is the eigenenergy or subband, inside the quantum well.
ϕ_i is the eigenfunction.

The proposed Hamiltonian, H, takes the kinetic energy operator and the effective potential energy (V_{ef}) terms are given by the band profile. Thus, one gets:

$$H = -\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m^*(x)}\frac{d}{dx} + V_{ef}(x) \qquad (2)$$

x is taken as the direction perpendicular to the epitaxial layers. Therefore, $m^*(x)$ is the position dependent effective mass. The effective potential V_{ef} is given by the band profile of figure 2, with experimental parameters taken from [8].

In particular, the eigenstates of the Schrödinger equation are calculated by using a split-operator algorithm [3,4,7], through a non-uniform finite difference discretization scheme, under the boundary conditions that the wave function must vanish at the substrate and the Schottky barrier.

3. RESULTS

Typical results from this procedures are exemplified in figure 3. It was plotted the quantum well profile (dotted line) and the probability density profile (continuous lines) of two electronic sub-bands. For clarity, these two functions are aligned with the respective sub-band energies (left scale).

The values of all sub-bands for electrons (EE) in CB and for the heavy (HH) and light holes (LH) in VB were calculated and are shown in Table 1.

Table 1. Sub-bands for electrons (EE), in CB, light holes (LH) and heavy holes (HH), in VB, for many well widths. The values are obtained considering the top of the well as reference (0,0 meV).

width (A)	EE (meV)	LH (meV)	HH (meV)
2.00	-53,740	-15,080	-46,218
2.25	-62,187	-18,036	-50,553
5.00	-125,280	-45,452	-73,238 -36,108
5.25	-128,808	-47,270	-74,155 -39,288
9.00	-160,709 -65,832	-65,060 -11,847	-81,241 -65,676 -40,657 -9,3666
9.25	-161,958 -70,138	-65,806 -13,673	-81,477 -66,595 -42,600 -12,101
9.50	-163,138 -74,2714	-66,514 -15,493	-81,697 -67,457 -44,431 -14,789
9.85	-164,685 -79,766	-67,449 -18,015	-81,983 -68,573 -46,817 -18,419
10.00	-165,314 -82,021	-67,830 -19,081	-82,097 -69,021 -47,781 -19,829
10.25	-166,318 -85,651	-68,441 -20,830	-82,278 -69,733 -49,314 -22,319
10.50	-167,273 -89,127	-69,023 -22,545	-82,449 -70,403 -50,762 -24,663
10.75	-168,179 -92,456	-69,579 -24,219	-82,619 -71,034 -52,130 -26,883
11.00	-169,0405 -95,6394	-70,109 -25,852	-82,760 -71,628 -53,424 -29,004

The possible transitions from electronic sub-bands, in CB, to heavy and light holes, in VB, are illustrated in figure 4 and calculated for all possible values in Table 2a and 2b.

Small variations like 0,25 nm in the well with could cause 13 meV of difference in the sub-band transition, for small wells (see the first two lines on Table 2a), but for larger wells, these sub-band transitions are from two to five meV.

Transitions from higher subbands (EEj, HHj and LHj with j equal to 2 or 3) of CB to higher subbands of VB are mostly affected by the changes in width of the well.

For wells of widths from the 2 nm to 10 nm, the mean variation is 3,5meV.

Table 2a. **Sub-bands transitions from electronic sub-bands (EE1) to light holes (LH) and heavy holes (HH) sub-bands for many well widths.**

well width (A)	EE1-LH1 (meV)	EE1-HH1	EE1-LH2	EE1-HH2	EE1-HH3	EE1-HH4
20	1731	1700				
22,5	1720	1687				
50	1629	1601		1638		
52,5	1624	1597		1632		
90	1574	1558	1627	1573	1598	1630
92,5	1572	1556	1624	1571	1595	1626
95	1570	1555	1621	1569	1592	1622
98,5	1568	1553	1617	1567	1588	1617
100	1567	1552	1615	1565	1587	1615
102,5	1565	1551	1613	1564	1584	1611
105	1564	1550	1610	1562	1582	1608
107,5	1562	1549	1607	1561	1579	1605
110	1561	1548	1605	1559	1577	1602

Table 2b. **Sub-bands transitions from electronic sub-bands (EE2) to light holes (LH) and heavy holes (HH) sub-bands for many well widths.**

well width (A)	EE2-LH1	EE2-HH1	EE2-LH2	EE2-HH2	EE2-HH3	EE2-HH4
90	1669	1653	1722	1668	1693	1725
92,5	1664	1648	1716	1663	1687	1718
95	1659	1644	1710	1658	1681	1711
98,5	1653	1638	1702	1651	1673	1702
100	1650	1636	1699	1649	1670	1698
102,5	1646	1632	1693	1644	1665	1692
105	1642	1628	1688	1640	1660	1686
107,5	1638	1625	1683	1636	1655	1680
110	1634	1621	1678	1633	1651	1675

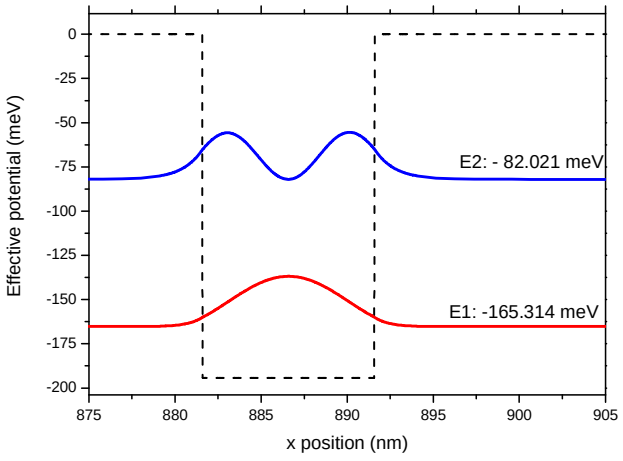

Fig. 3. Probability densities of the two only electronic states inside the quantum well of 10 nm width. The effective potential is the dotted line. Each density is aligned with its respective sub-band value, refereed to the top of the well (0 meV).

4. CONCLUSION

It was analyzed quantum wells from 2 nm to 11 nm.

The possible electronic transitions from de CB to VB were calculated, considering the calculated values of quantum sub-bands of electrons and holes and the band gap.

Uncertainties like 0,25 nm (typical value of one crystal monolayer) in the well width could give optical transitions uncertainties from few meV up to 13 meV, for small wells.

Of course, a more accurate study should be developed, but this study and numerical procedure could be a tool to this development, and these results are a warning to these quantum metrological area.

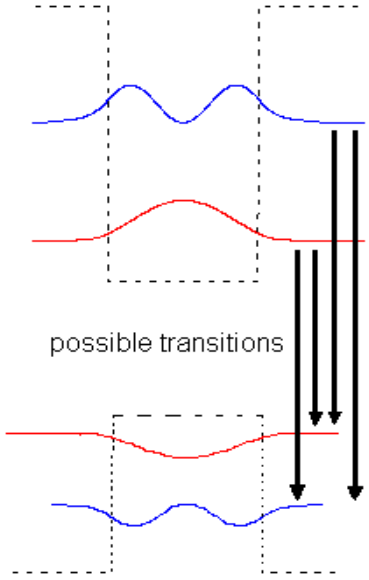

Fig. 4. Sketch of transitions from the electronic sub-bands to the light hole sub-bands.

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