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ELECTRONIC BAND STRUCTURE ENGINEERING OF SYNTHETIC SEMICONDUCTORS

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Abstract
A quantum well superlattice, built from two semiconductors, is a synthetic material whose new properties are only remotely related to the properties of the bulk semiconductors from which it is made. This paper deals with modeling of SC superlattice, as a key point in the development of new nanoscale electronic devices. In this work, we report results from the simulation of SC superlattice band structure using the transfer matrix method. It includes a comparative study of the transmission coefficient as determined by the shape of the heterostructure interface, with possible applications in synthesizing two contact nanoscale devices.
Keywords: superlattice, transmission coefficient, numerical simulation.

1. Introduction

Quantum well superlattices are receiving considerable attention due to their propensity to be used in nanoelectronics and photonics, as was envisaged [1]. There is a major interest in numerical computation of these devices, in order to tailor and optimize their operating properties. The majority of authors resort to a square quantum well (finite or infinite) description of confinement carrier potential, despite of their own consideration concerning interface width and roughness determination [2-4]. Actual technological applications of quantum wells construct non-abrupt interfaces, and it seem opportune to pursue an improved knowledge on the subject. The research is conducted for understanding the interface nature in nanometer scale and its role on the properties of ultra-small devices [5]. The effect of interface profile on the physical properties in non-abrupt quantum wells superlattice is addressed in this paper. Usually, the 2-D quantum wire and 3-D quantum dot can be reduced to the 1-D case using potential quantification by the multichannel method, as we do in our calculations.

2. Interface model and investigation method

In our investigations we focus on the transmission coefficient because physical properties (band structure) and electrical properties (by example the Landauer-Buttiker conductance) of the

nanostructures are directly related to it. The transmission coefficient has been computed via the transfer matrix formalism [6]. For the band structure of a superlattice the Kramer condition [7] has been used: $\left|Tr(\mathbf{M})\right| \le 2$ (1)

where **M** is the transfer matrix for basis-cell in the infinite superlattice, as it was defined in [6]. The mathematics of the Schrodiger equation has been reduced to a simplified matrix algebra and a piecewise constant potential approach.

A simplified nanostructure of double-barrier resonant-tunneling (DBRT) structure $Al_xGa_{1-x}As/GaAs$ with parameters as depicted in fig.1, has been chosen for input in numerical computation. The interface model is based on the existence of graded transition layers, with width *a*, which are responsible for smooth change from wells to the barriers. Three cases have been analyzed, when the Aluminum content *x* at interface is assumed of linear, parabolic and atan like-type, respectively. Also, the potential, *V*, and electron effective mass, m_e^*, will have the same shape because of linear relations to *x*. For example in conduction band: $V = 0.77x$ and $m_r = (0.067 + 0.083x)m_0$, where m_0 is the electron bare mass.

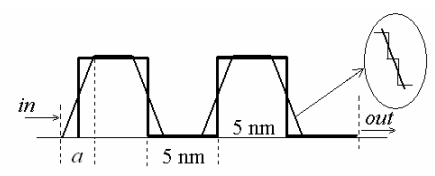

Fig 1. Schematic of $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ double barrier: the square (bold) and linear graded interface. The detail suggest the piecewise constant potential approximation used in numerical computation. The *in out* markers are for superlattice basis-cell.

In all numerical calculation $x = 0.45$. The initial well and barrier are 5 nm width and the higher barrier is $V_0 = 0.3465$ eV.

3. Results and Discussions

The numerical results are extracted from our research in the QUANET Project framework, devoted to transfer matrix method development for nanoscale device simulation.

Fig. 2a shows the transmission coefficient for the DBRT when the transition layer width *a* range linear from 0 nm (Heaviside like-type transition) to 2nm, in 25 steps of Al content, *x*, and $2.1 \cdot 10^4$ points for electron energy between 0 and 0.7eV. It can be seen a blue shift of tunneling channels and an increasing of transmission coefficient above the higher potential barrier V_0 with relaxation of transition layer. Detail inside show a remarkable tunneling energy change in prediction over to 10 meV. The algorithm has been proved convergent at $a = 0.01$nm (not shown

in fig. 2a) when for the linear and square x variation, the transmission curve are superimposing. Fig 2b depicts also a numerical convergence study related to *x* sampling for piecewise constant potential (*a* = 1nm). It follows that the convergence criteria are met for n greater than 20, case in which the curves remain quasi the same. Fig 3c show the influence on transmission coefficient from spatial change in heterointerface composition. Apart from the linear variation, a red shift of tunneling channels occurs when the variation is quadratic or atan functions. At energies greater than Vo, a parabolic-type connection produces an increase of the transmission coefficient while a natural connection (atan-type) produces an decrease.

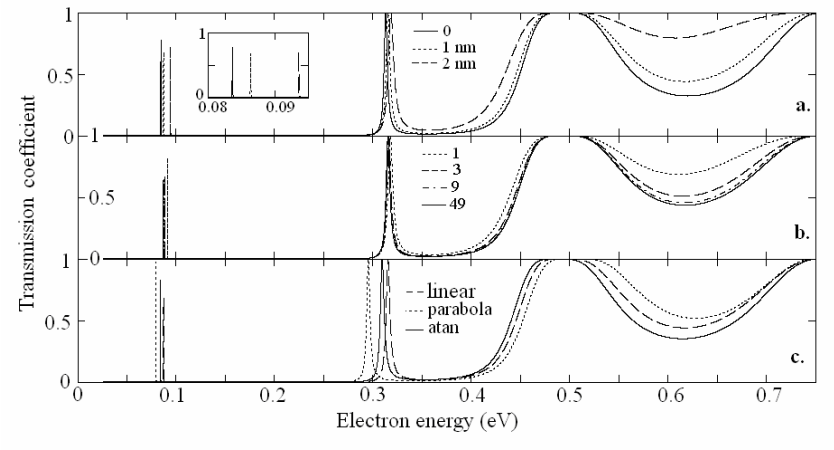

Fig 2. Transmission coefficient through DBRT structure in fig 1, with parameters: width of transition layers (a), the number of steps for Al content in transition layer (b) and interface shape determined by the stoichiometric composition.

In Fig. 3 we plotted the transmission coefficient for the case of linear coupling of 20 DBRT cells in a superlattice structure. We can deduce a similar behavior to that of the basis cell, but additionally we see a widening of the mini-bands with decreasing raccordation slope.

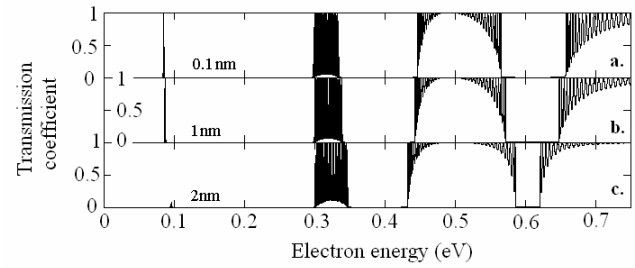

Fig 3. Transmission coefficient for a superlattice when the Al content at heterointerface vary linear in a transition layer wide of 0.1nm 1nm, 2nm.

Fig. 4 depicts the band structure as determined by condition (1) for the DBRT application as basis cell in an infinite superlattice when Al content has a linear, atan, quadric and square root of 3rd order dependence. For every case band calculation has been done for transition layer widths *a* between 0.1 and 2 nm in 0.1 nm steps. At first sight, a clear dependence of the allowed energies with the nature of the connection is observed, also essential different behaviors for each different

situation. With the exception of parabolic-type connection, for all other situations we find that a blue-shifting of the tuneling energy and a spectral widening that goes with parameter *a*, occurs. The most stable connection type regarding fluctuation of *a* (transition layer width) is found to be for the arc-tangent shape.

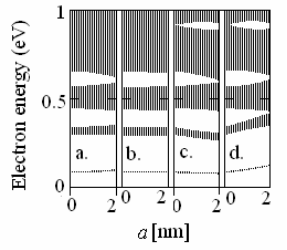

Fig 4. Band structure of an infinite superlatice with DBRT basis-cell. Allowed electron energy versus transition layer width, when the Al content spatial variation is: linear (a), atan (b), quadric (c), square root 3rd order (d).

4. Conclusions

This work substantiates considerable effects of the heterojunction interface shape on the properties of quantum well structures. As many simulations are done using the Heaviside interface approximation it is advisable to be careful with the results. On the other hand it emerges that precise control of all details of the transition layer means gaining control over opto-electronical properties of the device.

Acknowledgements

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References

[1] J.M. Martinez-Duart, R.J. Martin-Palma, F. Agullo-Rueda *Nanotechnology for micro-electronics and optoelectronics* Elsevier Ed, 2006.

[2] P. Harrison, *Quantum wells, wires and dots*, Wiley-Interscience Ed, 2006.

[3] M Shen, W Cao *J Phys D*, **33** (2000) 1150.

[4] H. Xu, *Physical Review B* 47, (1993) 9537.

[5] J.S. Sousa, G.A. Faris, V.N. Freire, *Superlattice and Microstructures* **25**, (1999) 377.

[6] M. Paulescu, E. Tulcan-Paulescu, P. Gravila, *Buletinul Stiintific al UPT*, **51** (2006), 95.

[7] P. Pereyra, E. Castillo "Theory of finite periodic systems: General expression and various simple and illustrative examples" *Phys. Rev. B* vol. 65, pp. 205120, 2002.