EMAC 2003 Proceedings

Proceedings of
The Sixth Engineering
Mathematics and Applications
Conference

University of Technology, Sydney
Australia, 9–11 July, 2003

Editors: R.L. May and W.F. Blyth

ISBN 1 86365 533 6

Preface

This volume contains papers to be presented at the Sixth Engineering Mathematics and Applications Conference (EMAC 2003) to be held at University of Technology, Sydney on July 9–11, 2003.

This conference is the sixth in a series which began with AEMC94, AEMC96, EMAC'98, EMAC 2000 and EMAC 2002. Like its predecessors, EMAC 2003 is held under the auspices of the Engineering Mathematics Group (EMG) (a special interest group of the Australian and New Zealand Industrial and Applied Mathematics division of the Australian Mathematical Society) and Engineers Australia. This conference is embedded within the International Congress of Industrial and Applied Mathematics (ICIAM 2003), and marks the change from even to odd years.

As can be seen from the Table of Contents, the papers in this volume are arranged in alphabetical order of first author. The full version of all papers appearing in this volume have been peer reviewed by two referees. In most cases both referees were members of the Technical Committee, but in some instances where some special expertise was required, other referees were used. The Editors would like to thank all of the referees, and particularly the members of the Technical Committee, for their efforts and valuable comments.

Finally we would like to thank our colleagues on the Conference Committee for their support.

Rob May
Bill Blyth

June 2003

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CONTENTS

Modelling Pyramidal Quantum Dot Nanostructures

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1 Introduction

Semiconductor structures can be fabricated with practically unlimited flexibility, and the formation of self-assembled quantum dots have been demonstrated in several different materials. These low dimensional structures, where the electron motion is confined from all three dimensions, are expected to play a pivotal role in many micro- and nano-optoelectronic applications.

The size and shape of such "quantum islands" depend substantially on the growth conditions and the technique used. In this paper we are interested in truncated pyramidal quantum dots, a class of quantum dots which attracted a substantial attention of experimentalists [10]. Although there have been studies of electronic bandstructures in these devices with tools of mathematical modelling and computational experiments [2, 3], up until now most such studies excluded the wetting layer from consideration. A systematic methodology for such studies has been recently proposed in [8]. However, the focus of the previous work has been on conical quantum dots.

2 Geometrical Considerations: Quantum Dots with Wetting Layer

The importance of the geometry in studying nanostructures has been emphasised in a number of papers (see, for example, [4]). By now, it is known that the variation in the dot size and shape can produce significant energy fluctuations in the strong confinement region (see, for example, [3, 7] and references therein). In this paper, we are interested in the analysis of truncated pyramidal quantum dots which are grown with the Stranski-Krastanov methodology from strained material systems [5]. The dot (that can be grown just a few nanometer in diameter) and the semiconductor matrix (in which the dot is embedded) are made of lattice-mismatched semiconductors. An important feature of the present work is that the quantum dots are considered together with the wetting layer. We base our consideration on InAs/GaAs structures. Our major focus is given to quantum dot structures of truncated pyramidal shape with wetting layer. A schematic representation of such quantum dot structures is given in Figure 1.

In what follows we will analyse numerically how eigenstates, in particular the ground and first excited states, in quantum structures are affected by the wetting layer. First, we will follow the line of [8] in finding eigenstates of what we call a "pure" quantum dot, that is the quantum dot without wetting layer. In this case, the layer of thickness "b" in Figure 1 is removed. These results are then compared with the results obtained for the quantum dot with wetting layer. We also analyse in detail the eigenstates of the wetting layer itself. The cone approximation of pyramidal quantum dots is then relaxed to the truncated pyramidal case. For this more realistic approximation, banstructures of three different quantum dots are reported.

3 Mathematical Model

In this paper, the effective mass methodology is used to formulate a Schrodinger type model. Such a model is derived based on the $\mathbf{k} \times \mathbf{p}$ methodology [8] and in the case of cylindrical symmetry can be written in the following form

$$-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left(\frac{1}{m_e(z,r)}\frac{\partial \psi}{\partial z}\right) - \frac{\hbar^2}{2}\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r}{m_e(z,r)}\frac{\partial \psi}{\partial r}\right) + \frac{\hbar^2}{2m_e(z,r)}\frac{n^2}{r^2}\psi(z,r) + V_e(z,r)\psi(z,r) = E\psi(z,r), \tag{1}$$

where $\psi(z,r)$ is the electron envelope function, E is the electron energy, $\hbar$ is Planck's constant divided

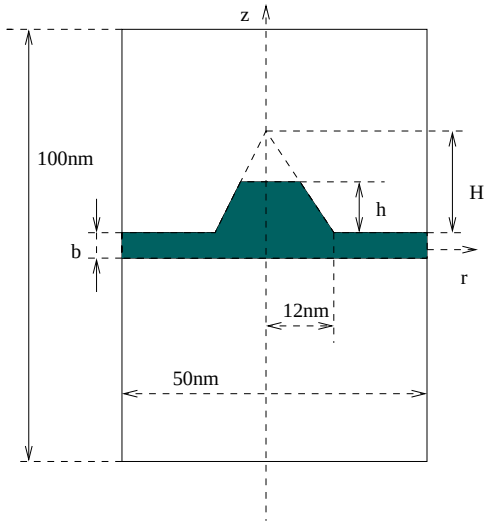

FIGURE 1. A schematic representation of the geometry of quantum dots under consideration.

by 2π, $m_e(z,r)$ is the position-dependent electron effective mass, $V_e(z,r)$ is the position-dependent band-edge potential energy.

From a mathematical point of view, the problem can be seen as an eigenvalue PDE problem. However, it is important to emphasise that both the original model and the derived model (1) have discontinuous coefficients due to different material properties in the quantum dot/wetting layer structure and the barrier. Hence, model (1) should be understood in a generalised sense.

From a physical point of view, one has to view the model (1) as such where the following two conditions should be satisfied (see, for example, [1])

$$\psi(z,r) \in C(Q),$$
$$-1/m_e^s \nabla\psi(z,r)\cdot\vec{n} = 1/m_e^b \nabla\psi(z,r)\cdot\vec{n}, \quad (2)$$

where $m_e(z,r) = m_e^s$ is the electron effective mass in the quantum-dot/wetting-layer structure, $m_e(z,r) = m_e^b$ is the electron effective mass in the barrier material, Q is the spatial (r,z) domain of interest, C is the class of continuous functions, and $\vec{n}$ is outer normal vector in the domain under consideration. Under these circumstances numerical methodologies based on a variational re-formulation of the governing equations is a natural tool in the analysis of these low-dimensional semiconductor structures as soon as realistic geometries and the wetting layer presence are included into consideration. Moreover, it should be noted that a special attention should be paid to deriving correct boundary conditions for the entire structure (see Figure 1). This issue has been addressed in [8] in detail, and here we use boundary conditions derived in [8] based on the Ben Daniel-Duke problem. Then, the problem is reformulated in a variational form, and is discretised by using a finite element approximation.

4 Computational Experiments

Before proceeding to this analysis of bandstructures of quantum-dots with wetting-layers, we make several remarks on discretisation of the developed model and its computational implementation. As we have already mentioned, from a mathematical point of view, model (1) supplemented by corresponding boundary conditions is a PDE eigenvalue problem. By using the finite element methodology, the problem is discretised. This leads to a large algebraic eigenvalue problem which is solved here with an efficient iterative procedure. More precisely, the corresponding algebraic eigenvalue problem,

$$(A-(E-V)I)\vec{\chi}_n = \vec{f} \quad (3)$$

with given matrix A and $\vec{f}$, is solved with the spectral transformation Arnoldi iterations (see, for example, [9, 6] and references therein). This Krylov-subspace methodology allows us to deal efficiently with the (large) matrix A resulting from the discretisation, by constructing iterations with respect to a sequence of spaces (m is the order of the corresponding Krylov subspace)

$$K_m(A,\vec{\chi}_n) = \mathrm{span}\{\vec{\chi}_n, A\vec{\chi}_n, ..., A^{m-1}\vec{\chi}_n\}. \quad (4)$$

To ensure a high accuracy of the results, computations were carried out on a sequence of grids, and all results reported here remain the same after further mesh refinement. The range of computed eigenvalues was specified within the limit given by the barrier energy level. This reduces the computational cost of the problem solution.

4.1 Quantum dots without wetting layer. Our first group of computational experiments follow the line developed originally in [8]. In all computations discussed below the height of the conical dot is $H = 3\mathrm{nm}$. In Figure 2 we present results for $n = 0$ where we observe two states both of which are confined to the dot region. Away from this region the eigenfunctions of these states decrease exponentially quickly in GaAs. Two eigenvalues corresponding to the ground and the first excited states are -0.2482 and -0.0189, respectively.

4.2 Quantum dots with wetting layer. The situation may change drastically if we add the wetting layer which is always present in experimentally grown nanostructures. For the wetting layer of thickness $b = 2\mathrm{nm}$ these changes are twofold. Firstly, the complete structure (quantum dot with wetting layer) has four eigenstates. Secondly, the actual values of energies for the ground and first excited states are substantially affected by the presence of the wetting layer, which is confirmed by values -0.4203 and -0.3005, respectively. Wavefunctions associated with these states are presented in Figure 3.

In the terminology of [8], both of the considered cases are confined to $n = 0$ and $k = 0$.

4.3 Analysis of the wetting layer. The above results show that a more detailed analysis of eigenstates in the wetting layer is required. Apparently the increasing number of states observed in the previous case is due to the presence of the wetting layer. Indeed, four eigenstates are observed for $n = 0, 1$, and 2. With the increasing n the number of eigenstates becomes smaller (three for $n = 2$ and 3; two for $n = 4, 5$, and 6), eventually leading to just one confined state (n = 7,8,9,10,11). We also observe that in terms of the actual values of energies, the ground states of the quantum well wetting layer exhibit a parabolic dependency with increasing values n. Finally, in Figure 4 we present wavefunctions for ground states of the quantum dot wetting layer for $n = 0$ and $n = 1$ (left and right upper figures, respectively), and both eigenstates for $n = 4$.

4.4 Truncated pyramidal quantum dots. To analyse the influence of the wetting layer on these structures, we first evaluate eigenstates of truncated pyramidal structures without wetting layer. We observe that the energy of such nanostructures decreases (in absolute

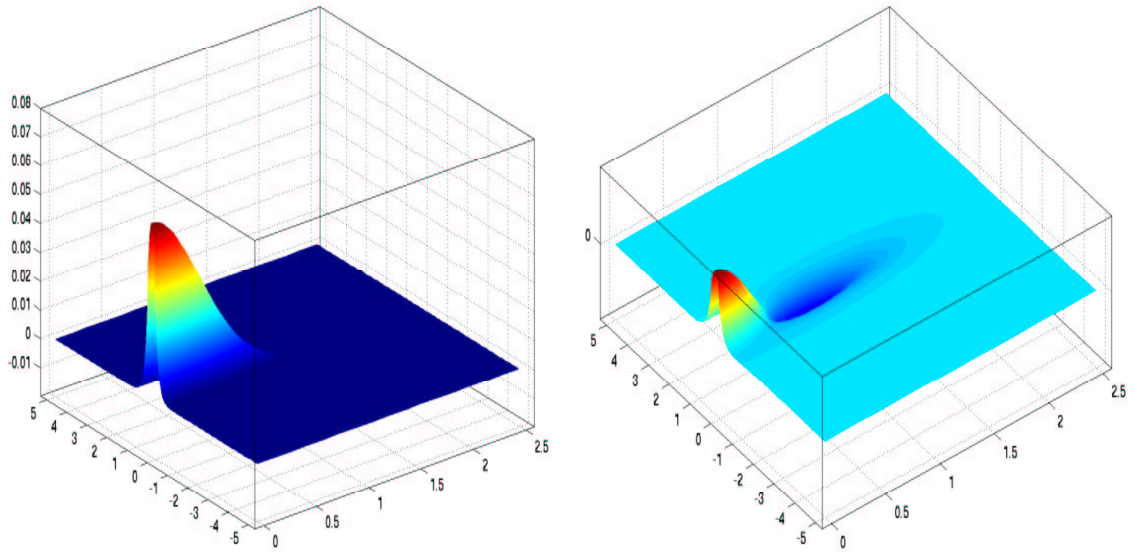

FIGURE 2. Wavefunctions of the ground (left) and the first excited (right) states for the conical quantum dot without wetting layer.

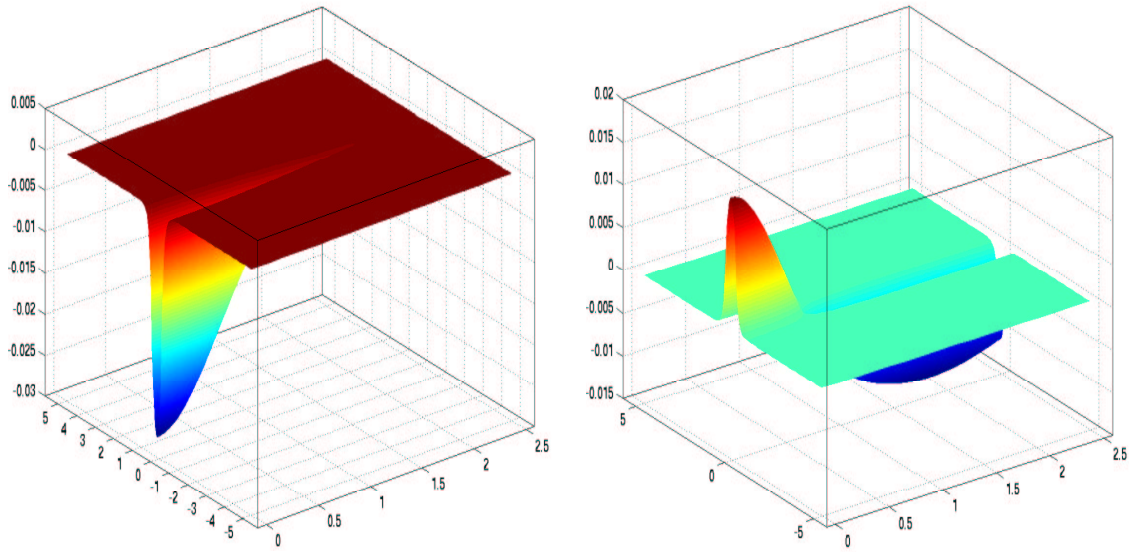

FIGURE 3. Wavefunctions of the ground (left) and the first excited (right) states for the conical quantum dot with wetting layer.

value) with decreasing height (h) of the truncated pyramidal dots. In Table 1 we present these observation in a quantitative manner. Note also that for small heights (see, for example, $h = 1$nm) only one confined state is observed.

In Figure 5 we present wavefunctions associated with both eigenstates (the ground and the first exited) of the truncated pyramidal quantum dot of height $h = 1.5$nm. Again, the actual energy values (-0.1780 and -0.0028) are substantially modified if the wetting layer is taken into account.

The number of eigenstates increases to four for all three quantum dot geometries analysed. The actual energy values for truncated quantum dots with wetting layer are given in Table 2, and wavefunctions associated with the ground and the first excited states of dots with height $h = 1.5$nm are presented in Figure 6.

Finally, in Figure 7 we present the results of com-

Truncated pyramidal dots without wetting layer		
Height 2nm	Height 1.5nm	Height 1nm
-0.2250	-0.1780	-0.1068
-0.01018	- 0.0028	

TABLE 1. Energy levels of the truncated pyramidal quantum dots without wetting layer.

Truncated pyramidal dots with wetting layer		
Height 2nm	Height 1.5nm	Height 1nm
-0.4142	-0.3998	-0.3755
-0.3057	- 0.3047	-0.3032
-0.2516	-0.2462	-0.2396
-0.1491	-0.1451	-0.1404

TABLE 2. Energy levels of the truncated pyramidal quantum dots with wetting layer.

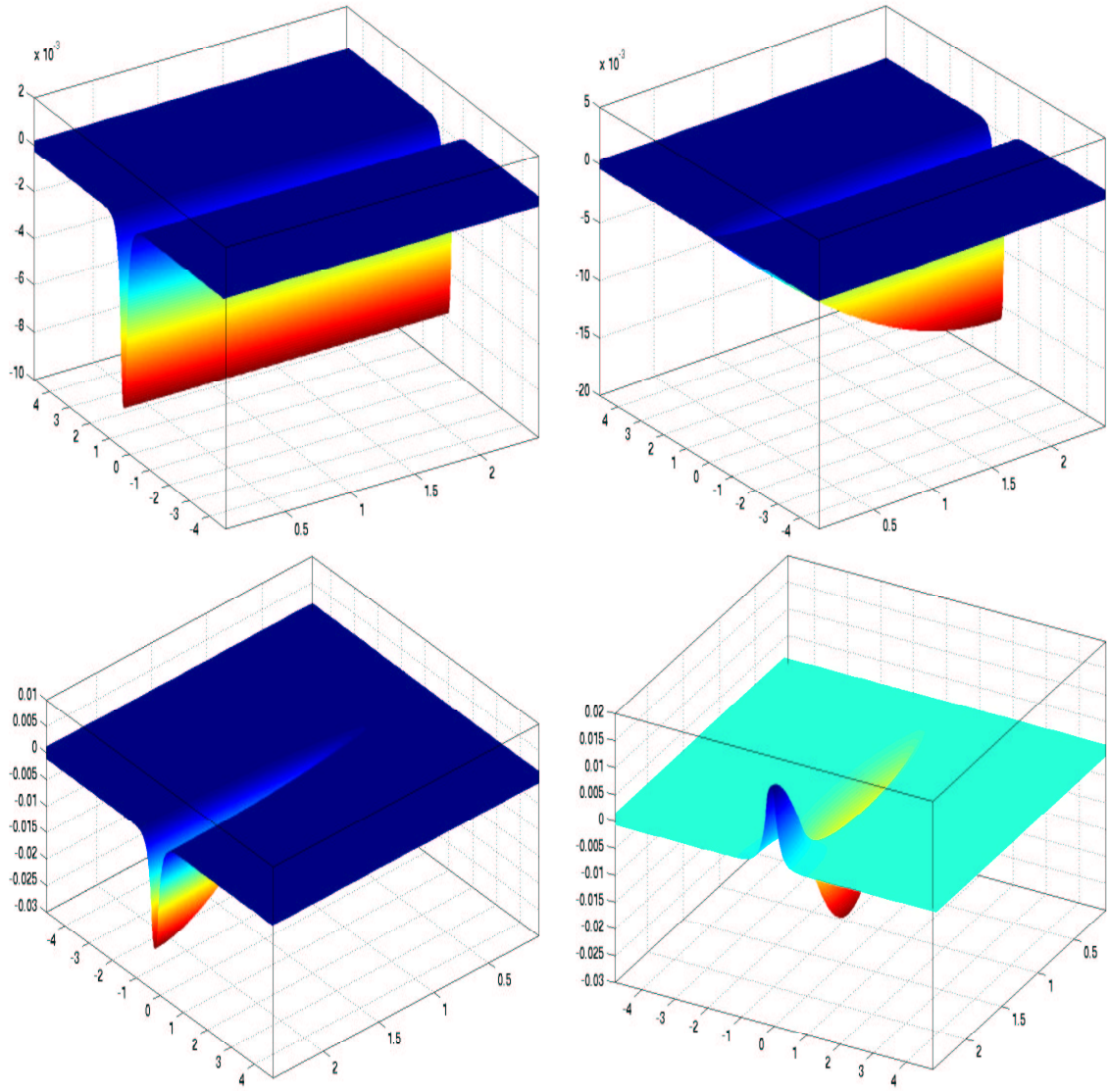

FIGURE 4. Wavefunctions of the quantum well wetting layer: ground states for $n = 0, 1$ (upper plots) and the ground and the first excited states for $n = 4$ (lower plots).

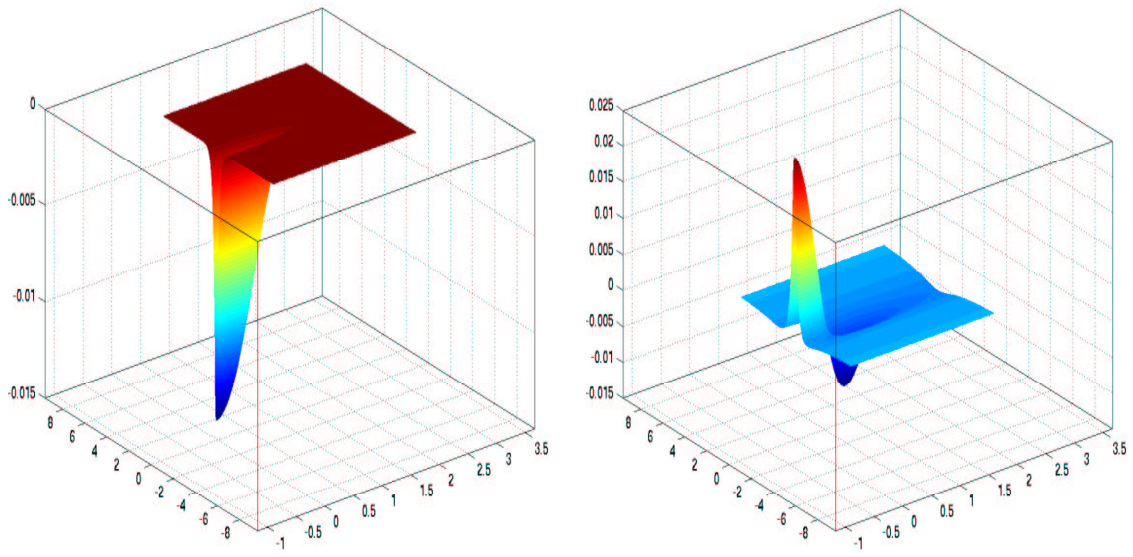

FIGURE 5. Wavefunctions of the ground and the first excited states in the truncated pyramidal quantum dot without wetting layer ($h = 1.5$nm).

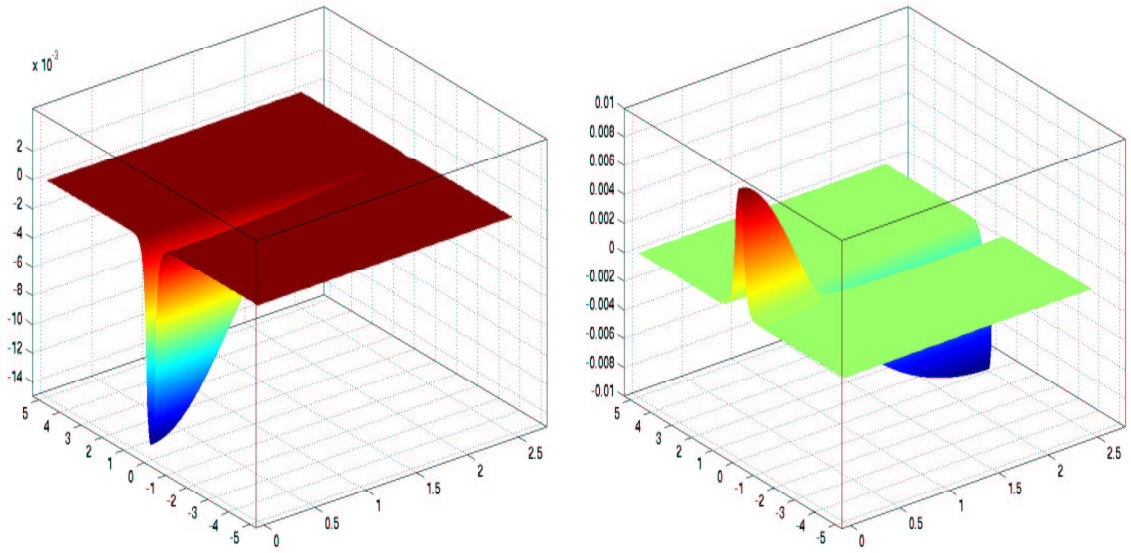

FIGURE 6. Wavefunctions of the ground and the first excited states in the truncated pyramidal quantum dot with wetting layer ($h = 1.5$nm).

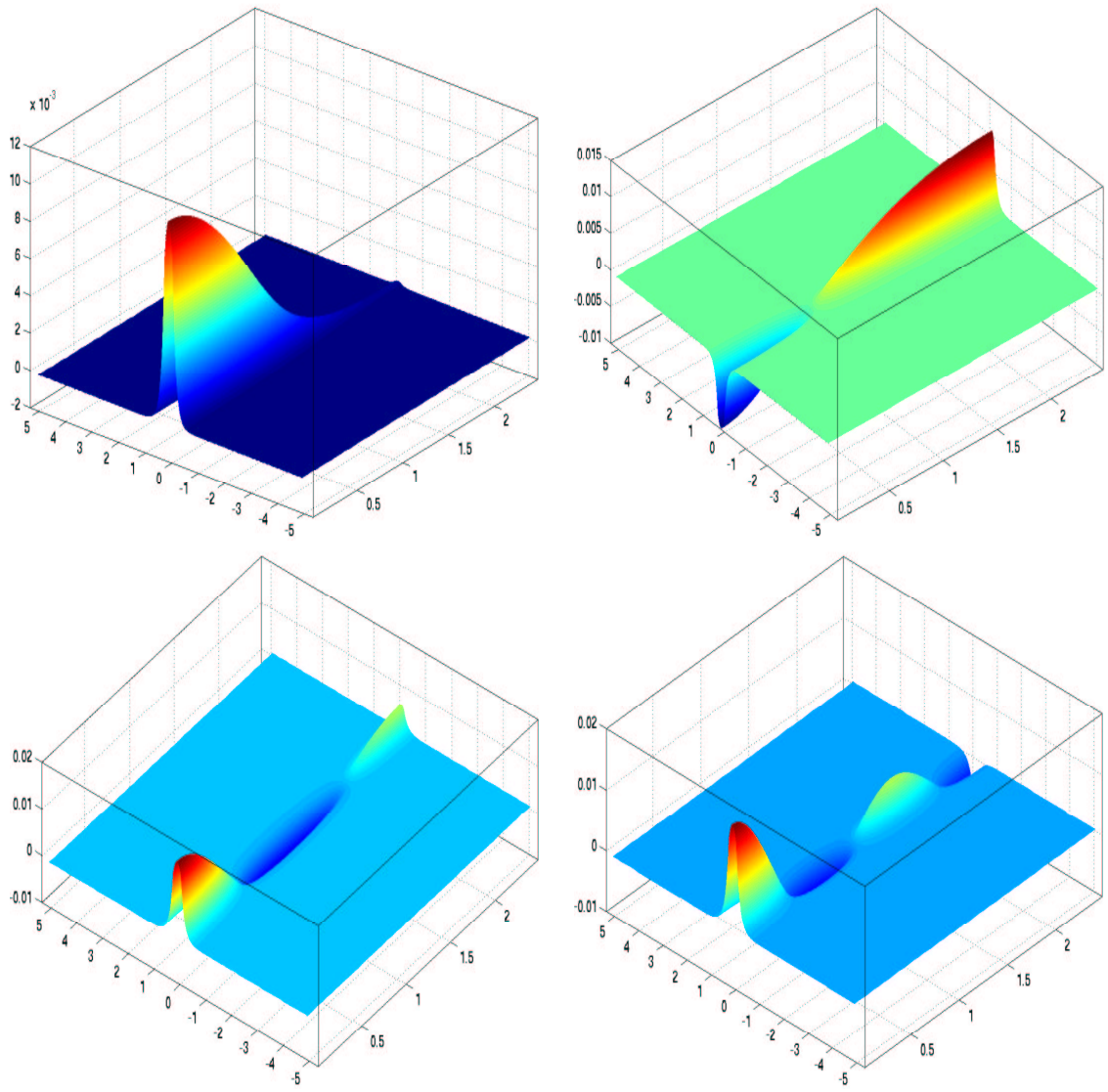

FIGURE 7. Wavefunctions of the ground and the first excited states in the truncated pyramidal quantum dot with wetting layer ($h = 1$nm).

putations of all four eigenstates for the truncated quantum dot with wetting layer of height 1nm. In this case, only the ground state is a confined dot state, yet even in this case the influence of the wetting layer can be clearly observed. All other states show an intrinsic coupling and state interference.

5 Conclusions

In this paper we analysed how the variation in the dot shape may affect energy fluctuations in confinement regions. Our major focus was given to the analysis of truncated pyramidal quantum dots which are grown experimentally. We demonstrated an essential interference between quantum dot/wetting layer states. For quantum dots that are intended to be used as active regions in the new generation of electronic and optical devices, the observed effects, originated from the quantum dot/wetting layer coupling, should be taken into account.

6 Acknowledgements

The author thanks Dr M. Willatzen for fruitful discussions on the topics of this paper.

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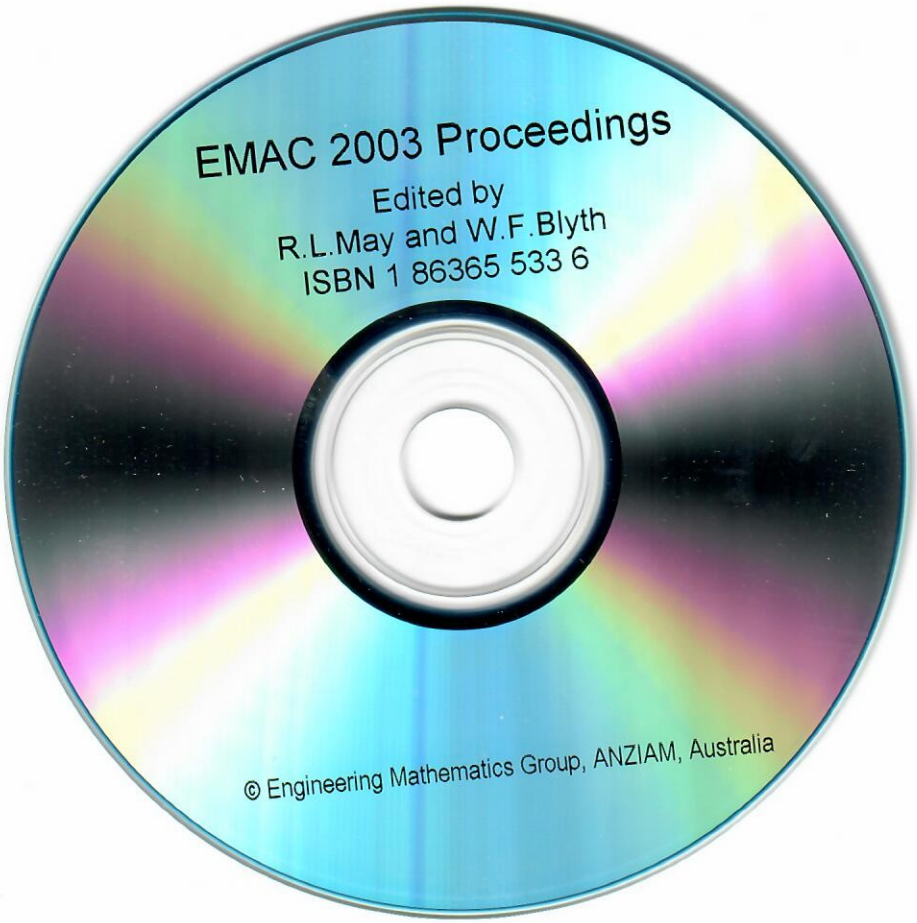
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