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On the existence of localized states in quantum pillars

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We have investigated the localization of electrons in quantum pillars, i.e. in nanometric structures in which electrons are confined by 5 sides, but are free to communicate with a bulk substrate of the same material through the 6th side and hence can be considered as open from this side. All nanopillars produced by an etching top-down process conform to this physical model. At first sight, electrons in such structures should have an equal probability of being everywhere, so confinement effects and consequently band-gap changes should not be present. However, experimentally, confinement effects are observed. We show, by a proper effective mass equation analysis of the combined pillars and substrate system, that eigenstates with a high degree of localization exist in the pillars – irrespective of the height of the pillar. Moreover, the eigenenergies of these states are extremely close to the energies of the quantum boxes that would be produced if the pillars were closed by all six sides. This analysis provides the justification for the previous application of effective mass calculations on the pillars alone.

1. Introduction

Quantum pillars are nanometric size semiconducting structures residing on a bulk material or film [1–7] of the same composition. In particular, Green et al. [1] have produced pillars on GaAs,

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Nassiopoulos et al. [2] on Si, the mesoporous Si by Canham et al. [3] consists essentially of nanoforests of Si wires on Si. Very recently ZnO nanorods have been produced by Willander et al. [4] and Cao et al. [5], InP nanopillars by Paramanik et al. [6] and GaN nanopillars by Chang et al. [7]. Optical absorption and emission experiments on these structures have revealed definite quantum confinement effects, such as band-gap widening. This widening depends on the size of the pillar and may vary from tenths of an eV to meV. In our view, however, such quantum confinement effects should not be so obvious at first sight for the following reason. Such structures are in fact bounded by 5 sides. Therefore, electrons in these structures are free to communicate with the bulk or film material below them and consequently they should have a wavefunction expanding in the substrate supporting the quantum pillars. Hence the localization of these electrons is not so obvious and neither are the quantum confinement effects, although they do experimentally exist as already stated. It must be emphasized that the above arguments apply to nanopillars that are produced by an etching top-down process which leaves the pillar–substrate interface intact.

In this paper we study this problem by a strict effective mass Schroedinger equation, which can allow a spill-over of the wavefunction into the substrate and we do indeed show that there are states in which the 5-sized bounded electrons may be approximately described by 3-Dimensional (3D) localized states irrespective of the height of the pillar. In particular, because the spill-over is "small" (small to be defined later in a not so obvious way), their quantum confinement effects are possible.

The phenomenon of wavefunction confinement in a space not fully closed by a potential barrier from all points of its surrounding surface is not new. It has been analysed by Weisshaar et al. [8] as well as by Sheng and Xia [9,10] for a waveguide with constrictions along its surface, by Akis et al. [11] for open quantum dots and by Tigelis et al. [12] for highly porous Si, which is essentially composed of undulating Si wires. In [8–10], a conduction problem is treated so that there are incoming, reflected and transmitted waves in an electron waveguide. Here the system sits at equilibrium prior to illumination. However, there is a direct connection since the localized states here are the ones that give zero conductance at an applied bias. We will come back to this point in the next section.

For quantum pillars there has been a previous work attempting to analyze wavefunction confinement [13]. However, zero wavefunction boundary conditions were imposed on the sides of a finite small substrate and hence one may argue that the obtained localization is a result of the imposed confinement in the substrate below the pillar. In this paper we impose periodic boundary conditions on the *xz* and *yz* planes of the unit cell of an infinite substrate (see Fig. 1), so that any localization that we obtain inside the pillar is a result of the pillar itself.

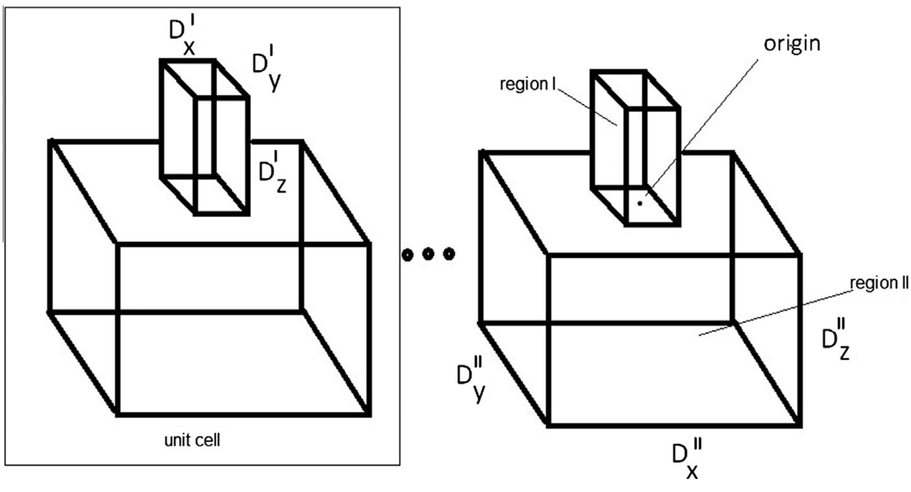

Fig. 1. Geometry of the structure under consideration.