NOVEL APPROACH TO THE FABRICATION OF ORDERED ARRAYS OF QUANTUM WIRES

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We propose a novel method for the engineering of one-dimensional nanostructure fabrication with no need of catalyst agents. The method is based on a lithography design of a pattern of channels onto a conveniently cleaved semiconductor surface, as illustrated in Fig.1. We believe that this method opens a range of possibilities for optoelectronic nanodevices with improved efficiencies.

We demonstrate by means of first-principles electronic structure calculations that when the channel diameter is sufficiently larger than the interstitial space, the resulting pillars constitute an ordered array of electronically independent, though mechanically interconnected nanowires. We also show that a controlled coupling of the nanowires can be achieved, as long as one is capable to tune, at fabrication time, the thickness of the interconnections, which are ultimately responsible of the efficiency of the quantum confinement. This method, being based on a top-down approach, would yield an ensemble of identical nanowires, grown along the same crystallographic orientation and with similar properties concerning the length and the diameter.

We present density-functional calculations [1] of different templates, where the channels – and consequently the nanowires – are distributed according to a square or a hexagonal network, discussing the case of silicon and gallium arsenide. The hexagonal distribution of channels proved to offer the best confining properties, while there is no clear evidence that any of these two materials should be clearly superior to the other for what concerns the confinement properties. Calculations have been performed with the Siesta ab-initio package [2]. For a silicon substrate, holes in a square disposition, wire size of 23.3Å and interconnects 22.0Å long and 5.5Å, we observe that states remain in the wire section. However, widening the interconnect to 11.0Å, we observe the appearance of laterally propagating states (see Figure 2). The dispersive behaviour is conclusively determined from the observation of the band width for the bands of interest (cf. Figure 3).

We also present results for structures with less demanding (i.e. bigger) feature sizes. Figures 2.d) and 2.e) show the charge density associated to the minimum of the conduction band for a GaAs substrate with different channel radii. These results are obtained with the Effective Bond Orbital Model (EBOM), and display d) purely 1D or e) two-dimensional superlattice behaviour.

The use of such structures could be easily extended to quantum well or superlattice substrates, e.g. GaAs/InGaAs or GaAs/GaAsP, leading to the fabrication of one-dimensional heterostructures or quantum dots with potential applications as light emitting devices.

References:

[1] R. Rurali, J. Suñé and X. Cartoixà, Appl. Phys. Lett., *in press*.
[2] J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón and D. Sánchez-Portal, J. Phys.: Condens. Matter **14** (2002) 2745.

Figures:

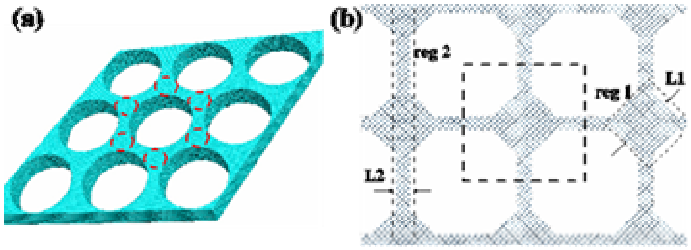

Figure 1 (a) Schematic of the proposed approach and (b) unit cell for the square topology.

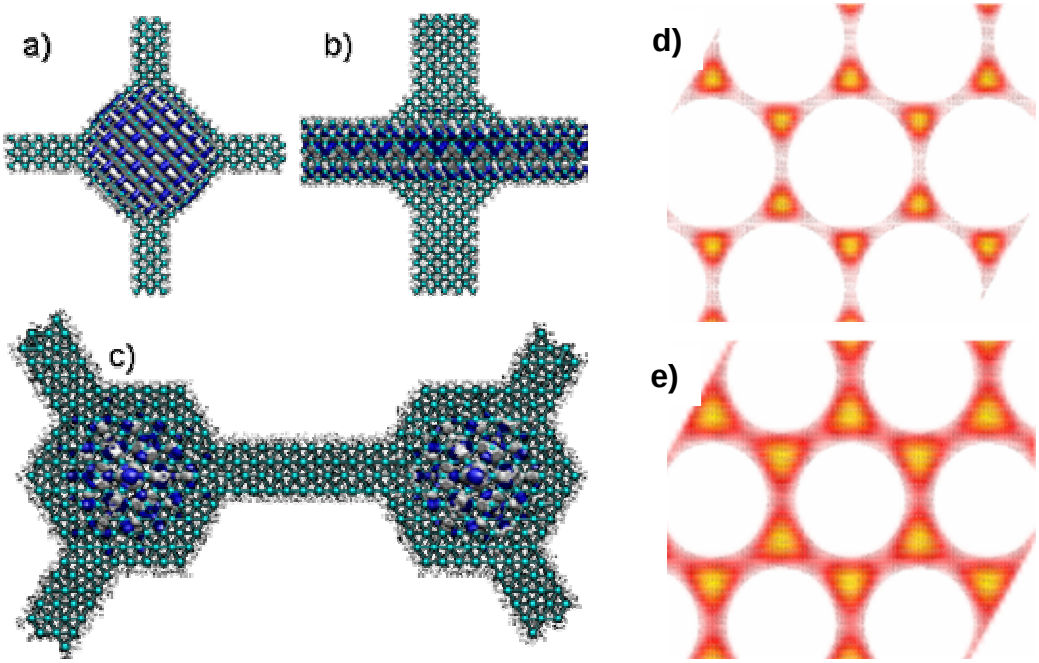

Figure 2 Wave-function of the lower state of the conduction band in the case of square [a) and b)] and hexagonal [c)] arrays of channels in silicon (unit cell shown). The confined character of the state sustaining the electron carriers is evident in a) and c), while b) is obviously propagating. Hole carriers are hosted by states with similar features (not shown here). d) [e)] shows isolated (interacting) NW behavior in GaAs, with a distance of 40 nm between hole centers.

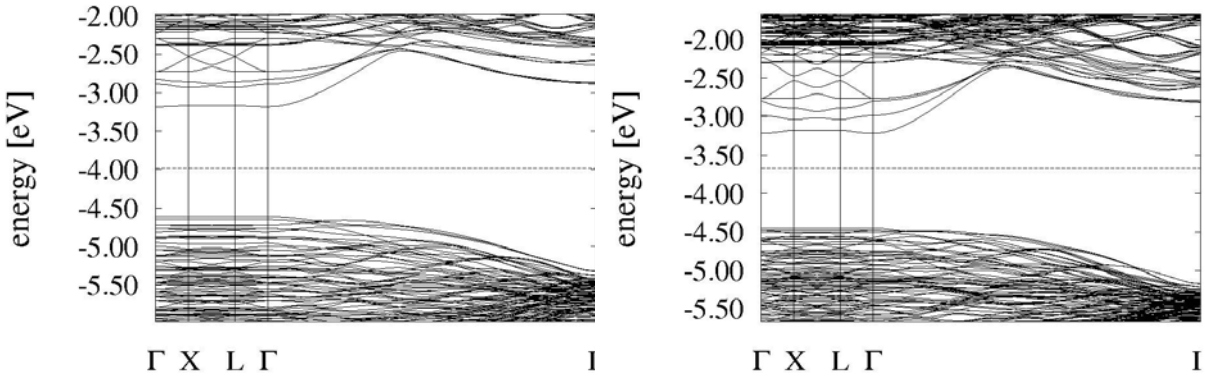

Figure 3 Band structure diagrams in the case of a square arrangement of channels in GaAs. The interconnections between neighboring pillars have a thickness of 0.6 nm (left panel) and 1.2 nm (right panel). With the thinner interconnections the bands disperse essentially only along k_z direction, indicating an efficient confinement; coupling between neighboring pillars starts to appear for the thicker interconnections.