

Comparison of the electronic structure of InAs/GaAs pyramidal quantum dots with different facet orientations

Jeongnim Kim,* Lin-Wang Wang, and Alex Zunger
National Renewable Energy Laboratory, Golden Colorado 80401

*Received 24 December 1997!

Using a pseudopotential plane-wave approach, we have calculated the electronic structure of strained InAs pyramidal quantum dots embedded in a GaAs matrix, for a few height (h)-to-base(b) ratios, corresponding to different facet orientations 101°, 113° and 105°. We find that the dot shape -not just size! has a significant effect on its electronic structure. In particular, while the binding energies of the ground electron and hole states increase with the pyramid volumes (b^2h), the splitting of the p -like conduction states increases with facet orientation (h/b), and the p -to- s splitting of the conduction states decreases as the base size (b) increases. We also find that there are up to six bound electron states ~12 counting the spin!, and that all degeneracies other than spin, are removed. This is in accord with the conclusion of electron-addition capacitance data, but in contrast with simple $\mathbf{k}\cdot\mathbf{p}$ calculations, which predict only a single electron level. @S0163-1829-98!50516-4#

Growth of semiconductor quantum dots via controlled coarsening of lattice-mismatched films¹ produces coherently strained islands. These “self-assembled” dots, capped by another semiconductor, exhibit rich spectroscopic features, including explicit evidence of quantum-confinement,² size and shape effects on the spectrum,^{3,4} emission from higher excited states,

boundary conditions in all three principal directions. We use
@100

\$101% and \$113% faceted dots, while it also has significant amplitude in the barrier for the \$105% faceted dots. The shape

faceted dot. On the other hand, we find three transitions,
 $C_s \rightarrow V_1, C_s \rightarrow V_2$

$P_x \sim \langle C_s | P_x | V_j \rangle$, $P_y \sim \langle C_s | P_y | V_j \rangle$, and $P_z \sim \langle C_s | P_z | V_j \rangle$ where x, y and z denote the $[100]$, $[010]$, and $[001]$ directions, respectively. We find the following:

~a! For the $[100]$ faceted dots, the transitions from the ground electron state C_s to the ground hole state (V_0) and to the excited hole states (V_1 and V_2) are allowed. Their transition dipole moments strongly depend on the polarization: the $C_s \rightarrow V_0$, $C_s \rightarrow V_1$, and $C_s \rightarrow V_2$ transitions are allowed for polarization P_x , P_z , and P_y , respectively.

~b! For the $[111]$ faceted dots, the transition from C_s to V_0 is forbidden (dark exciton!), while it is allowed for $[100]$ and $[110]$ faceted dots.

~c! There are no dipole-allowed transitions polarized along the z direction (P_z transitions!) for the flatter $[100]$