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Alberto Franceschetti and Alex Zunger

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Free-standing versus AlAs-embedded GaAs quantum dots, wires, and films: The emergence of a zero-confinement state

Alberto Franceschetti and Alex Zunger
National Renewable Energy Laboratory, Golden, Colorado 80401

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Using a plane-wave pseudopotential method we investigate the electronic structure of free-standing and of AlAs-embedded GaAs quantum dots, wires, and films. We predict that ~i! the confinement energy of the valence-band maximum ~VBM! is larger in AlAs-embedded than in free-standing quantum structures, because of the zero-confinement character of the VBM wave function in the latter case; ~ii! small GaAs quantum structures have an indirect band gap, whereas large GaAs quantum structures have a direct band gap; ~iii! the conduction-band minimum of small free-standing quantum structures originates from the GaAs X_{1c} valley, while it derives from the AlAs X_{1c} state in AlAs-embedded quantum structures; ~iv! the critical size for the direct/indirect crossover is larger in embedded quantum structures than in free-standing quantum structures. © *1996 American Institute of Physics.* @S0003-6951~96!02124-9#

Semiconductor nanostructures have received great attention in recent years, both from an experimental and a theoretical point of view. Several techniques have been developed to confine carriers in two or three dimensions, leading to the realization of quantum wires and dots. The two general strategies commonly used to realize quantum confinement rely on ~i! embedding the semiconductor quantum structure in a larger-gap semiconductor barrier ~e.g. GaAs in AlGaAs or InGaAs in GaAs!, or ~ii! using an organic solvent to create a confining barrier for the semiconductor quantum structure. In the former case ~embedded quantum structures!, effectivestead that the VBM envelope function is almost constant for $(\bar{1}10)$ quantum films, and that the G_{15v} Bloch-periodic wave function nearly vanishes at the boundary of the quantum film, automatically satisfying zero boundary conditions. In the case of AlAs-embedded films the VBM energy *does* depend on the film thickness, and the VBM envelope function has the usual sine-like form predicted by the effective-mass approximation ~Fig. 2!, thus explaining the larger confinement energy of the VBM state.

A wave-function analysis shows that the CBM of free-standing GaAs quantum films originates from the bulk X_{1c}^{z} valley for L , 8 ML, while it becomes a G_{1c}-derived state for L . 8 ML ~see also Table I!. The direct/indirect crossover is evident in Fig. 1~a! as a kink of the energy vs thickness curve at L ; 8 ML. In AlAs-embedded thin films, on the other size dependence of the VBM energy. Nevertheless, the VBM confinement energy of AlAs-embedded wires is still slightly larger than the VBM confinement energy of free-standing wires ~for $L > 5$ ML!. The CBM of free-standing quantum wires originates from the GaAs X_{1c} valleys for thicknesses

up to L 5 14 ML ~28 Å!, while it becomes a G_{1c}