Strain-induced interfacial hole localization in self-assembled quantum dots: Compressive InAs/GaAs versus tensile InAs/InSb

Lixin He, Gabriel Bester, and Alex Zunger*

National Renewable Energy Laboratory, Golden, Colorado 80401, USA

Using an atomistic pseudopotential approach, we study how the shape of the dot (spherical vs lens shaped) affects the position-dependent strain and the electronic properties of tensile sInAs/InSbd and compressive sInAs/GaAsd quantum dots. We compare the strain profiles, strained modified band offsets, confined levels, and atomistic wave functions of these dots. We show (i) how the existence of position-dependent strain in nonflat heterostructures can control the electronic properties, leading, for example, to interfacial localization of hole states on the interface of matrix-embedded dots and (ii) how the dots shape can control the level sequence and degeneracy. For example in spherical dots, one finds degenerate light-hole (LH) and heavy-hole (HH) states, whereas in lens-shaped dots one can have as the highest-occupied hole state either (a) a LH state inside the dot, becoming a HH state outside the dot sInAs/InSb tensile case) or (b) a HH state inside the dot, becoming a LH states outside the dot (InAs/GaAs compressive case).

I. INTRODUCTION

Semiconductor heterostructures[1,2] are often constructed from lattice-mismatched components (Si/Ge, InAs/GaAs, InAs/InSb). This leads, in general, to the creation of both isotropic (hydrostaticlike) strain $I = e_{xx} + e_{yy} + e_{zz}$, as well as biaxial strain $B = fse_{xx} - e_{yy}d^2 + se_{yy} - e_{zz}d^2 + se_{zz} - e_{xx}d^2g^{1/2}$, where e_{ab} are the ab

$$H_v(\vec{\varepsilon}) = H^{SO} + a_v I - D_{001}(\vec{\varepsilon})\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \qquad (8)$$

where $D_{001} = b_v(e_{zz} - e_{xx})$ is the heavy- or light-hole splitting or crystal-field splitting. The eigenvalues of this equation give the energy of the three valence bands VB1, VB2, and VB3 in decreasing order of energy. The strain-modified confining potential shown in Figs. 4 and 5 is obtained by solving Eq. (7) in real space at each eight-atom unit cell using the local strain input from VFF.

To analyze the valence confining potentials obtained from Eq. (7) in terms of their HH, LH and SO character, we project the eigenfunctions to the HH, LH, and SO basis sets, i.e., $|J, J_z\rangle = |3/2, \pm 3/2\rangle, |3/2, \pm 1/2\rangle, |1/2, \pm 1/2\rangle$, respectively. The dominant character of each band is marked in Figs. 4 and 5 as "HH," "Jl0""Jl0 (4)-268.7(272)9.8(⁄19 0 w-3002256ning)2t00225.1(con)Tj (en911-1.11 1 Tf 0.7057 0 s.17757 0 stmark(rkT

first three valence bands VB1, VB2, and VB3 are given for
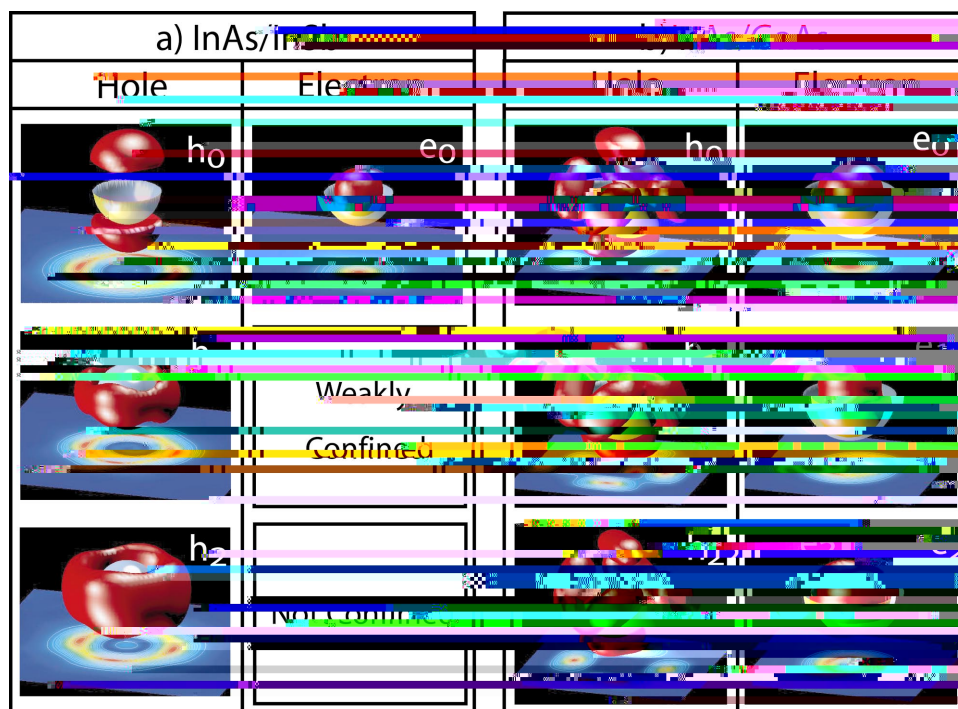the equatorial plane of the sphere. The first valence band

FIG. 7.