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tures: two-dimensional films, one-dimensional cylindrical
wires, and zero-dimensional spherical dots; all of these
cases are accessible to analytic treatment in the effective-
mass framework. In the case of an isolated GaAs quan-
tum structure embedded in A1As, we find that the critical
size for the onset of the I ~X transition is 31 A in a
two-dimensional quantum film, 56 A in a one-
dimensional cylindrical quantum wire, and 80 A in a
zero-dimensional spherical quantum dot. We also find
that the interaction between GaAs quantum structures
tends to reduce the critical size for the occurrence of the

I ~Xtransition. We further investigate the effects of the
alloy composition, finding that the critical size decreases
when the Ga concentration in the Al Ga& As matrix

increases. This is explained by the reduction of the po-
tential barrier at the GaAs/Al„Ga, As interface. In
the case of a spherical GaAs quantum dot embedded in
Al Ga& As, we show that, depending on the dot radius
and the alloy composition, different alignments of the
band-edge states lead to different regimes of the lowest-energy optical transition.

GaAs film in AlAs matrix

CBM

-3.70

- 3.80
(a)

-3.90

-4.00

AIAS GaAS. AlAs

1"1,(GaAs)

choosing E„fin the band gap, one obtains the band-edge states of the system, with the same accuracy achieved in a conventional diagonalization of the Hamiltonian. Since only the band-edge states are obtained, the computational

II. PSEUDOPOTENTIAL CALCULATIONS

A. Method

The pseudopotential method, providing a microscopic
description of the system, allows a straightforward
identification of the 1 ~x transition in GaAs/A1As
quantum structures. The total pseudopotential (ps) of the
system is given by the sum of screened atomic pseudopo-tentials centered at the atomic positions R„:

V~,(r)= g U„(r—R„).

- 5.50

C
-5.60

- 5.70

-5.80

I 15v (GaAs)

We have used the empirical atomic pseudopotentials developed by Mader and Zunger, fitted to measured in-terband transition energies, efFective masses, and defor-
mation potentials of bulk GaAs and A1As and to Prst-
principles wave

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effort scales linearly with the size of the system. The
minimization procedure is carried out in a plane-wave
basis set using a preconditioned conjugate-gradients algo-
rithm. Periodic boundary conditions are assumed at the
boundaries of a large super cell including the GaAs
domain and the A1As barrier. Because of the use of periodic boundary conditions, a residual interaction be-
tween the GaAs domains is inevitable. However, with
the choice of a sum. ciently thick barrier the convergence of the band-edge energies to the limit of isolated struc-tures is of the order of a few meV.

-3.70

-3.80

CBM

GaAs wire in A1As matrix

(b

B. Isolated GaAs quantum structures in pure AlAs

First we consider an isolated (001) GaAs quantum film
in an A1As matrix. Our pseudopotential results are
shown in Fig. 2 as a function of the film thickness I. For
GaAs films with thickness I & I, (where I, =28 A, or 10
ML's), the CBM energy of the heterostructure is almost degenerate with the X„energy level of bulk AlAs. An analysis of the CBM wave function for I & I, shows that this is actually an X-like state localized in the A1As bar-rier [insert (a) to Fig. 2]. For thicker GaAs films (I & I,) the CBM energy begins to drop as the film thickness in-creases, approaching the I &, level of bulk GaAs. In this region the CBM wave function has a strong I -like char-acter, and is localized in the GaAs film [insert (b) to Fig.
2]. Thus, the I ~Xcrossover is predicted to occur at the critical thickness k, =28 A, corresponding to 10 ML of
GaAs. The I —+X transition is characterized by a

+X

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GaAs quantum wires in A1As

d =45.3 A d = 56.6A

CBM 1 CBM 2 CBM

VBM VBM

FIG. 4. VBM and CBM wave-function amplitudes of GaAs
[001] quantum wires in A1As. The wave-function amplitude, averaged a1ong the wire direction, is plotted in the (001) plane. The solid circles denote cross sections of the GaAs wires (of di-ameter d). For d=45. 3 A the CBM is a double-degenerate X-like state localized in the A1As matrix. For d=56.6 A the CBM is a nondegenerate I -like state localized in the GaAs wire. In both cases the VBM is localized in the GaAs wire.

next section). Taking into account the thickness of the AlAs barrier necessary to decouple the quantum dots, we
estimate the size of the GaAs/AlAs system necessary to
observe the I ~X transition to be of the order of
-5X10 atoms. This is outside the range accessible to
pseudopotential calculations. A recently developed rnul-

tiband k.p method predicts a critical diameter d, =70 A for the I ~Xtransition in GaAs/AIAs quantum dots.

C. Interacting GaAs quantum structures in AlAs

To address the consequences of the interaction among

GaAs quantum structures for the onset of the I ~X
transition, we have performed pseudopotential calcula-tions for interacting quantum films and quantum wires. First, we consider a periodic array of (001) GaAs quan-
tum films embedded in AIAs (GaAs/A1As superlattice).
The array period (i.e., the distance between the central planes of two consecutive GaAs films) is kept fixed at a value L slightly larger than the transition thickness I, of a single quantum film, while the well thickness is varied from 0 to L. The results for L=34 A are shown in Fig. 2 (dashed line) as a function of the film thickness l. In com-parison to the case of an isolated GaAs quantum film in A1As, two new efFects arise: (i) for thin GaAs films the CBM energy is no longer constant, but initially increases with the filin thickness, and (ii) for thick GaAs films the CBM energy decreases faster than in the case of an isolat-
ed film. Thus, the I ~X crossover (identified by the
change of slope of the dashed line) occurs at a thickness smaller than the critical value l, for an isolated film; of

course, the exact value of the critical thickness depends on the array period L.
Similar results are obtained for interacting quantum
wires. In this case we have considered a square array of
[001]-oriented GaAs cylindrical wires embedded in an
A.1As matrix. The CBM energy shown in Fig. 3 (dashed
line) is obtained for a nearest-neighbor distance D= 57 A.
The reduction of the critical size for the I —+X transi-
tion can be readily interpreted in the framework of the
effective-mass approximation. As we can see from Fig. 1,
the X„state of bulk GaAs is higher in energy than the X&, state of bulk A1As, so the former acts as a potential
barrier for the latter. Thus, when the thickness of the
A1As barrier is finite, the Xi, state is pushed up by quan-
turn confinement. Furthermore, electrons bound to
neighboring GaAs quantum structures can interact,
lowering the ground-state energy, if the barrier is not too
thick. These two effects add up to decrease the critical
size for the onset of the I ~Xtransition.

III. EFFECTIVE-NIASS CALCULATIONS

While pseudopotential band-structure calculations pro-vide an accurate, microscopic method to obtain the criti-
cal size for the I ~X transition, they are not practical when the critical size is very large, such as in
GaAs/Al Gai „As quantum dots. For simple domain
geometries, on the other hand, the one-band effective-
mass approximation (EMA) provides a direct, analytic
method for calculating the transition size of GaAs quan-
tum structures embedded in an Al Ga, As barrier.
Our basic assumption is that an electron localized in a GaAs dorn. ain is confined by a potential barrier Vz corre-sponding to the energy difference between the I &, states
of Al„Ga, As and GaAs (see Fig. 1 for the x= 1 case).
In other words, we neglect the I -X mixing of the
conduction-band minimum when the latter is localized in

GaAs domains. The Schrodinger equation in the EMA is
solved by assuming the continuity of the envelope func-tion and of the current density at the boundary of the
quantum structure. The critical size for the I —+X transi-
tion is obtained by equating the confinement energy of
the electron to the energy difference V~ between the Xi, state of Al Ga, „As and the I „state of GaAs (see Fig. 1). At low Al concentrations (x (xo) the alloy band gap
is direct (Vi, (V~), and the I ~Xtransition of the CBM

is not possible. At high Al concentrations (x &xo) the alloy band gap is indirect (

domaif 35 (at)Tj ET BT /Xi3 9.34 TfT BT /Xi3 8.76 Tf 314.44 (2 Td (Xi3 23 Tf 42 BT /Xi3 8.87 Tf 385.wXi3 23 Tf 42 BT /Xi13 8.87 T519.56 2aj ET BT9j ET BT58 Tf 443.78 249.67 Td (I)Tjj ET BT /XT BT /Xi3Tf 443.11 2

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GaAs quantum structures in Al„Ga, „As

75

60

cn 45
cga V
30

15

0.25 0.50 0.75

Al concentration in barrier

FIG. 5. Critical size for the I —+X transition in
GaAs/Al Ga& As quantum films, wires, and dots, as a func-
tion of the Al concentration in the barrier, calculated by the effective-mass approximation.

TABLE I. Material parameters for bulk GaAs and A1As and for the Al Ga, As alloy used in the effective-mass calcula-tions. Here m is the I &, effective mass, Ez. and Ez are the I &, and X&, band gaps, br and b~ are the alloy bowing parameters for the I „and X&, band gaps, and hE»M is the valence-band offset of the GaAs/A1As heterojunction.

0

the case x=1, we obtain l, =31 A for a quantum film and d, =56 A for a cylindrical quantum wire. These results
should be compared with l, =28 A and d, =52 A ob-
tained from the pseudopotential calculations: the
difference is less than 10%, suggesting that in this size re-gime the EMA is a good approximation.
A detailed discussion of the applicability of the EMA
to heterostructures can be found in Ref. 10. Mader and Zunger" recently compared the one-band EMA with direct pseudopotentials calculations for (GaAs)„/(A1As)„ (001)

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PhTf 45Td (O.)Tj ET BT /ue7311 631.11 Td (1115iTd (edited)Tj ET BT 4e/ue7311 631.11 Td1.22 661.89 Td (3279)Tf 501.1111 71922 6S 362.44 630.89 Td79 8.36Lon5ld