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Empirical atomic pseudopotentials for A1As/GaAs superlattices, alloys, and
nanostructures

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with a

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tices of various orientations. (iv) We verified that the
wave function of bulk and superlattices obtained with
our pseudopotentials agree well with those obtained in
first-principles LDA calculations. To illustrate the util-

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Alo 5Gao 5As alloy, treated in the virtual-crystal approx-

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gebraic forms, one for the Ga, and one for the Al and As potentials. These functions were fitted to the discrete form factors of the bulk zinc blende solids. The L-like

band gaps of the (001) n x n superlattices are not given in Ref. 14, and the pseudodirect-to-direct crossover is not
determined. However, the I'-like gap at n = 10 is still
110 meV above the X -like gap and by extrapolation the crossover will probably be well above the experimentally found value of n 11.
All of the previously constructed empirical pseudopo-tentials for A1As/GaAs assumed a single As potential for both GaAs and AlAs, or used the two bulk band struc-

EPM

(010)

(AIAs), /(GaAs), (001)

Self-consistent LDA

(AIAs), /(GaAs) „(111)
Self-consistent LDA EPM

(a) RI Qu

FIG. 2. Comparison of (a) I'q, and (b) Rq, wave func-
tions squared of the (A1As) q /(GaAs) q [001] superlattice
(the "CuAu structure" GaAIAss) as obtained with the self-consistent LDA (left) and the empirical-pseudopotential method (right), respectively. The results are shown in the (010) plane, using the same contour level spacings [0.5
&)~ electrons/(a. u.)]

for both the LDA and the EPM wave func-

tions. Rq, corresponds to the folded zinc blende Lq, state and
is lower in energy than I'~,.

tures only. In short-period superlattices, however, a large &action of the As atoms is located at the interfaces. We believe that a local-environment dependence of the As potential such as given in Eq. (4), is crucial for the EPM to accurately reproduce the band structure in this regime (see Table III). Furthermore, a correct band offset and good effective masses are important for large-period. su-perlattices, and hence a correct prediction of the type-II to type-I transition.

IV. ILLUSTRATIVE APPLICATIONS

FIG. 1. Comparison of (a) f'I,, (b) I'~,, and (c) I'q
wave functions squared of the (AIAs)z/(GaAs)z [111]super-
lattice (the "CuPt structure" GaAIAss) as obtained with the
self-consistent LDA (left) and the empirical-pseudopotential
method (right), respectively. We plot the results on the (110) plane using the same contour level spacings [1 electron/(a. u.)]

for both the LDA and the EPM wave func-

tions. Diagonal lines denote the (111) planes. I'q„ is the
nondegenerate crystal-field split state originating from the
zinc blende I'z5 states. It is below the doubly degenerate

r.„state by A~F. f„and f, are the symmetry-repelled -(~) -(2)
conduction states originating from F~ and

I'q„

Lq, e 1844 T3.56 8j ET BT /Xi6 8.46 Tf 97dET 1.9eET u2Tf 277.78 650.65 Td nXi6 8.47 Tf 52.13 71.19 Td (splitting)Tj ET BT /Xi6 8.18 Tf 88.65 T 196 Td (energy)Tj ET BT /Xi6 8.26 Tf

apply present ef-

ficient is

neeT /Xi6 ET l81.89 T10.29 Tf 424 T3.200.36 T 27to

solTf 243.56 716.32 Td (the)7cti301 30354 Td 24 Td (Comparison)Tj ET BTIf 207.85 153.32 Td (ve)Tj ETi6 8. ET BT 2.69 133.07 Td (and)Tj 1 Tf 242n perlattic2 ET BT /433BT the a.

as

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TABLE IV. Comparison of previous EPM's vrith the present one. In the second column, the

potential type is specified, i.e., "atomic, " if atomic form factors are used [see Eq.(1)], "bulk, "
if the bulk potential of A1As and GaAs is retained aud au infinitesimal interface in A1As/GaAs is assumed. Columns three to Sve indicate whether deformation potentials aud the A1As/GaAs band ofFset were fitted, and how V(q) was obtained at those reciprocal vectors that are uot zinc blende vectors Gza (see text). The symmetry of the CBM of the n = 1 (A1As) /(GaAs) (001) superlattice is reported in the last column. Quasiparticle calculations (Ref. 44) place the n = 1 CBM at R(I).

Method Potential type

Caruthers and Lin-Chung va, vA~, vA,
(Ref. 12) atomic potentials

Def. pot.
6tted
No

AE
6tted
No

V(q) at

Interpolated

(001) SL
n, =1 CBM

I'(X,)

Andreoni et al.

(Ref. 13)

Av = v~& —vAl
bulk/atomic

No No Interpolated

Gell et aL

(Ref. 15)

AlAs, GaAs
bulk potentials

No Yes I'(X,)

Xia

(Ref. 14)

VCa, VA1, VAS

atomic potentials

No Yes Algebraic 6t f(X,)

Ikonic et al.

(Ref. 16)

AlAs, GaAs
bulk potentials

No Yes Convolution R(L)

Present Vaa1 VAl,
v~, [Ga4 „Al„]
atomic potentials

Yes Yes Algebraic fit
sup ercells

A. Superlattices with chemical interfacial roughness

Chemical nonabruptness of interfaces in short-period superlattices has been suggested4 as a reason for the discrepancy between the experimental assignment of the conduction-band minimum and theoretical predictions (see Table III). In particular,

is

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2.4

(AIAs) il(GaAs)i (001)

2.3-

Ov

2.1— I4,, M5

1.9-

(I)1c
1c

"ho 0.2 0.4

I

0.6 0.8

Degree q of CuAu LRO

FIG. 3. Spectral averages of the zinc-blende-like I'q, (di-amonds), Xq, (pluses), and Lq, (squares) energy gaps, re-spectively, plotted as a function of g, the degree of CuAu long-range order. The solid line is a quadratic interpolation between the rl = 0 and 0 = 1 values of (I'q,)

and the bro-
k

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microscopic potential and at the same time large super-
cells are needed. The experimental feasability of such
small nanostructures has been demonstrated recently,
e.g., by intentional MBE growth of Ino 5Gao 5As quan-
tum dots embedded in GaAs, and by unintentional for-
mation of GaAs "quantum dots" at the AlAs/GaAs in-
terface of A1As/GaAs quantum wells. s4 We illustrate the
usefulness of our present method for theoretical studies of
embedded quantum dots by considering substitutional n-
atom Ga clusters with idealized geometries in an AlAs
host crystal, denoted AlAs:Ga„, where n connected Al
atoms are substituted by Ga atoms. It is known that
a single Ga isoelectronic impurity (n = 1) in AlAs does not have a bound state in the energy gap. Very large
clusters may be described by the particle-ia-a-box, or
effective-mass model. In terms of the efFective-mass pic-ture, a GaAs quantum dot in A1As acts as a quantum well with a potential depth of about 1 eV. The xninimum size of a spherical quantum dot above which effective-mass theory predicts a bound electron can easily be cal-
culated to be n 160. However, the CBM of AlAs is
at the X point in the Brillouin zone rather than at the I' point, hence quasibound states with small binding en-
ergies can lie in the continuum of the A1As conduction
bands and will form resonant states even for very small cluster sizes. An analogous situation occurs in the case of ultrathin GaAs quantuxn wells in AlAs, where it was calculated that for (001) quantum wells with thickness d smaller than ll monolayers, the quantum-well states are
resonant with the AlAs conduction bands, and only for
d & 11 do bound electrons below the CBM exist. s

In the

case of a spherical quantum dot, a simple effective-mass
calculation gives a cluster size of n —4200 above which
a bound electron exists below the AlAs X edge. Here,
we are interested in much smaller cluster sizes, where
resonant electron states are expected.
To simulate a Ga„cluster in an AlAs host, we use a cubic supercell containing 512 atoms, which is sufBciently large to prevent interaction between the periodically re-peated clusters for small n. We then replace n = 1, 4, and 14 Al atoms by Ga, taking the shape of cubic cluster geometries, i.e.,

for n = 4 we have a tetrahedron and for
n = 14 we have a cube. We can classify the eigenstates of the systems according to molecular orbitals of cubic
point symmetry. In Fig. 5 we plot the near-band-edge
spectra of the substitutional clusters as a function of the efFective supercell composition x = n/256. For all clus-ters considered, we 6nd the lowest unoccupied state to be an X-derived threefold degenerate t2 level. This state is clearly not effective-mass-like. In fact, inspection of
the wave function for n = 14 reveals that this t2 state

is AlAs-like, i.e.,

it is extended in the A1As region and
slightly attenuated in the GaAs cluster. Therefore, we identify this state with

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TABLE V. Same as Table

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Note that because the EPM uses screened atomic poten-
tials, the absolute reference energy of the solid is simply
that of the free atom.

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We have used

a kinetic-energy cutoff for the plane-wave ba-
sis of 5.0 Ry, resulting in about 30 plane waves per atom. The potential V(r) was discretized on

a simple-cubic grid
with

a resolution b,

r
= a/12, where

a

= 10.68 a.u. is the
GaAs and A1As lattice constant. This grid resolution cor-responds to a maxium momentum q in reciprocal space of 3.53 a.u.

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