PHYSICAL REVIEW B VOLUME 50, NUMBER 23 15 DECEMBER 1994-I

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

Kurt A. Mader and Alex Zunger
1Vational Reneisable Energy Laboratory, Golden, Colorado 80/01 (Received 2 June 1994; revised manuscript received 31 August

17 394 KURT A. NADER AND ALEX ZUNGER

with a

50 EMPIRICAL ATOMIC PSEUDOPOTENTIALS FOR A1As/GaAs... 17 395

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-

17 398 KURT A. MADER AND ALEX ZUNGER 50

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

EMPIRICAL ATOMIC PSEUDOPOTENTIALS FOR A1As/GaAs...

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

KURT A. MADER AND ALEX ZUNGER

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

50 EMPIRICAL ATOMIC PSEUDOPOTENTIALS FOR A1As/GIAs... 17 401

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

KURT A. NADER AND ALEX ZUNGER

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

EMPIRICAL ATOMIC PSEUDOPOTENTIALS FOR A1AS/GaAs... 17 403

TABLE V. Same as Table

50 EMPIRICAL ATOMIC PSEUDOPOTENTIALS FOR A1As/GaAs.

.

. 17 405

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

J. van Laar, A. Huijser, and T. L. van Rooy, J. Vac. Sci. Technol. 14, 894 (1977).
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.

T. C. Chiang, J. A. Knapp, M. Aono, and D. E. Eastman, Phys. Rev.

B 21, 3513 (1980).
D. D. Sell, Phys. Rev.

B B, 3750 (1972).
D. E. Aspnes, C. G. Olson, and D. W. Lynch, Phys. Rev. Lett. 37, 766 (1976).
A. R. Goni, K. Syassen, K. Strossner, and M. Cardona, Semicond. Sci. Technol. 4, 246 (1989).
K. Reimann, M. Holtz, K. Syassen, Y. C. Lu, and E. Bauser, Phys. Rev.

B 44, 2985 (1991).
D. Olego, M. Cardona, and H. Muller, Phys. Rev.

B 22,
894 (1980).
A. Azema, J. Botineau, F. Gires, and A. Saissy, J. Appl. Phys. 49, 24 (1987).
J. M. Chamberlain, P. E. Simmonds, R. A. Stradling, and G. G. Bradley, in Proceedings of the 11th Interna tional Conference on Physics of Semiconductors, Warsaw, 197g, edited by M. Miasek (PWN-Polish Scientific, War-saw, 1972), p. 1016.
M. S. Skolnick, A. K. Jain, R. A. Stradling, L. Leotin, J. C. Ousset, and S. Ashkennazy, J. Phys.

C 9, 2809 (1976).
A. F. Kravchenko, W. S. Sardarjan, and W. W. Efimov, in Proceedings of the 8th International