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(vi) We predict that ordering can significantly enhance
the degree of spin polarization of electrons photoemitted
kom the VBM. Ordered III-V alloys can thus be used
as
a good polarized electron source. These general re-
sults open avenues of band-gap engineering by combin-ing epitaxial strain with atomic ordering. Experimen-tally testable predictions are made and summarized in Sec.

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(2 o 0) (I o 0) f

1 o 0)
H„= av —bv. 0 1 0 e~~+ 0 —2 0 6yy+ 0 1 0 ~zz
0 0 1) (

0 0 1) (

0 0 —2)

(O —10) —~3d„—1 0 0 e „+ (o o o)

o o 0) $

o o —1)
0 0 —1 e„,+ 0 0 0

0 —1 0) (

—1 0 0) &zx (6)

t

1 0 0

Hooi „—a„+—Aooi(e) 0 1 0
(0 0 —2)

(7)

In this case E1 and E2 are degenerate, while E3 is sep-arated &om E1 and E2 by the crystal field splitting 6osoi(e), which is given by
S
Boo, = 3b„[e„——e~~].

For (111) strain we have from Eq. (2) e = e»
e„and e „=e„, = e,, so the second term in Eq. (6)
vanishes, and the Hamiltonian becomes

(

0

+ +alii(e)

(

—1 —1 0

Again, in this case E1 and E2 are degenerate while E3 is separated Rom E1 and E2 by the crystal field splitting b,iii(e), which is given by

3~3d1I cap (10)

The solutions of H give three energy levels, E1,E2, and E3 for each strain. As will be illustrated next, this Hamiltonian can be further simplified for strain parallel to the high symmetry [001] or [111]directions.
For (001) strain we have from Eq. (2) e = e» g e„ and e „=e„, = e, = 0, so the third term in Eq. (6)
vanishes. The Hamiltonian becomes

B. Pure atomic ordering

It is now known that vapor-phase growth of most
III-V zinc-blende semiconductor alloys results in sponta-neously ordered structures. Most of these ordered struc-
tures can be characterized as superlattices. For example,
the ordered Cupt-like structure is an alternate mono-

layer superlattice along the G,s

s

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P(x, rl) = P(x, o) + rl' [P(X, 1) —P(X,0)], (12)

provided that the property can be well expressed in terms
of single-site and pair interactions.

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In our definition e is negative (positive) for in-plane com-
pression (tension). From Eq. (17) the conduction-band
energy relative to the center of the top valence bands is
given by

E,(e) = E,(0)+2a e. (22)

11

The Hamiltonian for the top of the valence states can be obtained by combining Eq. (7) with Eq. (15), i.e.,

1 H„=—3

(+001

-~so

0
0
0

S
+001
0
0
0

0
0
—2400
~SO
i~SO
0

0
0
ISO
S
+001

0

0
0
~SO
ISO
S
+001
0

~SO
~SO
0
0
0

2+ooi)

where the crystal 6eld splitting is

~S () = 3bC11+ 2| 12

11

(24)

Diagonalization of Eq. (23) gives three spin degenerate eigenvalues of the in-p/ane light-hole (lh) [I's„, (j 3/2, mi = +3/2)], heavy-hole (hh) [I'r„, (j = 3/2, m& —— +1/2)], and spin-orbit split-off (SO) [I'r„, (j = 1/2, m@ —— +1/2)] states. Here, we use the notation of Ref. 21. Note that along the [001] direction the roles of light-hole and heavy-hole are reversed. Explicitly,

E'"() = —3[&' +&'-()] 1

E'"() = -6[&"+&o'o ()] 1
~SO + ~S ~

2 QSO~S

E (e) = ——[6 + b,ooi(e)]

1

~SO + ~S ~

2 ~SO~S

For systems

with

to

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ture elastic constants C;~ and deformation potentials a
and b for the III-V semiconductor compounds GaP, InP,
GaAs, and InAs. Using Eq. (28) we give also n and P
for the four compounds show in Table I. We have also
calculated o. and P directly from Eqs. (26) and (27) us-
ing the first-principles linearized augmented. plane wave (LAPW) method within the local density approxima-tion (LDA). The calculated T = 0 values ct.1,DA and Pr, DA are given in Table I. We find that the calculated I.DA values are systematically smaller than the exper-imental values measured at room temperature. This could be due to the strong temperature dependence of the band-gap deformation potential. For example, for GaAs, a at T = 120 K is about 3 eV smaller than at room temperature. This, in turn, will reduce o. and P by the same magnitude

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spin-orbit splitting we use the bowing 6~so ———0.02
eV, while for the direct band gap the bowing

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100

(a)

Ordered Ga„ln, „P/GaAs (001)
I I I I I I
I

(b) „ 0 4

Ordered Ga„ln, „P /GaAs (001)
80 I I I I I I I I

(a) . (b)
60-

-0.6

)

—100

LJj

-200— I

I
I

Xp
I
I

I I I I

0.40 0.45 0.50 0.55 0.6 0
Composition x

I I I I I I

0.2 0.4 0.6 0.8
Ordering Parameter g

~ 40 E
CV

LJJ

&I

20

0 50 100 150

—AE (x) (meV)

0 100 200 300

-hE,(g) (meV)

FIG. 7. Band-gsp reduction b,E~[g, e(z)] = E~ [il, e(z)] E~[0—, 0] of the strained Gs Ini, P alloy as s function of (s) composition z snd (b) long range order parameter g. The experimental data of Ref. 35 are plotted as solid dots in (b).

80

(a)
60—

~ 40 E
CV

Lj
20

Ordered Ga„ln, „P/GaAs (001)
I I I I I I

. (b)

Xp

o.4o 0.45 o.5o o.55 0.6 o

0

Composition x

0.2 0.4 0.6 0.8
Ordering Parameter g

FIG. 8. Valence-band splitting RE~2 of the strained Gs Ini P allay as s function of (s) composition z snd (b) the long range order parameter g. The experimental data of Ref. 35 are plotted as solid dots in (b).

This strain e(z) is a function of the film composition z, and so are the other composition-dependent properties

P(z) for the strain-free random alloy. We use Vegard's

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strain-free

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6'

) 0. We thus have the

I 6,

—I'6„and the

I 6,

—I'7„ tran-
sitions. For pure (001) strain both transition

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(v) Optical transition intensity analysis can be used to

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