EPITAXIAL EFFECTS ON COHERENT PHASE DIAGRAMS OF ALLOYS 4063

II. CONTINUUM ELASTICITY PICTURE OF COHERENT EPITAXIAL ENERGETICS

A. Elastic description of

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1 for h&h,
S(h)= '
y(2 —g) for h ~ h„ (2.6)

B. Qualitative eÃects of epitaxy
on phase stability and coexistence

To illustrate how the epitaxial constraint can selective-ly stabilize certain structures, consider the schematic solid-state reaction between solids a and f3 to produce an ordered or disordered phase a,P,

xa+ (1—x)/3+~a, P, (2.7)

where y(h)=(h, /h)[1+in(h/b)]/[1+in(h, /b)] is the
fraction of the misfit accommodated elastically, and b is the Burgers vector of the relevant misfit dislocation. Thus the total epitaxial strain energy of the partially coherent epitaxial film decays to zero with a characteris-tic 1/h dependence for large h, as shown schematically in Figs. 1(c) and 2. In practice, activation barriers against nucleation of such dislocations in semiconductors permit coherent growth considerably beyond the equilibrium value of h,.

a, =a,q[a„13t „]. Since EEs(a„P&)=0 in this case,
bEEs(a,)

~ 0 and 5H,~(a,) ~ EHbk. If bulk and epitaxial entropies are similar (as we demonstrate below), the cor-

responding change in free energy I also obeys
5F,~(a,) (AI'bk, so that the reaction proceeds more com-pletely epitaxially than in bulk. The two generic cases are 5H p

& 0 and 5H, p

)a.
I. 5H,q &0

If bHb&)0 (common if n and P are isovalent semicon-
ductors) but bEEs bHbk one may promote a reac- 40 tion epitaxially even ifit does not occur in bulk. Case (i) is
shown schematically in Fig. 2(a), whose left-hand side
shows energies of bulk and thin epitaxial films. Effect (i) of the Introduction is a manifestation of epitaxial stabili-zation of an ordered compound with respect to decompo-sition into its coherent constituents. Such an eA'ect was predicted

"

for a rhombohedral SiGe compound on a Si
substrate, for

'

chalcopyrite Ga2AsSb, ZnHg Te2,
GaInP2, and ZnCdTez, and for CuAu-I-like GaInP2, all
on lattice-matched substrates. Epitaxial stabilization of
unusual structures [effect (ii) in the Introduction] may
If the reaction takes place incoherently in bulk with no applied pressure, all three species a, 13, and a„P, „are ree to adopt their equilibrium lattice dimensions a, [a], a, [P], and a, [a P&], respectively (neglecting bulk coherency strain, discussed in Sec. VID). The bulk for-mation enthalpy is defined as the change in zero-pressure enthalpy in this reaction:

[8] —BEE &AHbk ~0; nP is lattice matched

Thin

epi.

b H k(x)=E, [a P)]XE.,

[n—]—(1 x)E.,[P].—
(2.8)

If, however, the

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be understood as selection of the structure with the small-est 5H, for a given a„as for CdTe in the rocksalt structure and zinc-blende MgS on substrates lattice matched to the novel (not the bulk equilibrium) phase. The right side of Fig. 2(a) schematically shows the thickness dependence of the energies of such an epitaxial-ly stable phase aP and its constituents a+P with disloca-
tions included. Since a13 is lattice matched to the sub-strate, its energy is constant for all film thicknesses h; by contrast, a+It is

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III. CLUSTER DESCRIPTION OF BULK
AND EPITAXIAL ALLOYS

A. Limitations of a continuum description

TABLE I. Bulk formation enthalpy AH {kcal/fcc-sitemol),

0

equilibrium lattice parameter a,q

{A), and cubic elastic con-
stants {CxPa) for Cu4 „Au„ordered compounds.

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0

TABLE II. Bulk formation enthalpy AH (kcal/fcc-sitemol), equilibrium lattice parameter a,q

(A),

and cubic elastic constants (GPa) for Ga4As4 „Sb„ordered compounds. Values for n =0,4 from zinc-blende structure, for n =1,3 from luzonite structure, and for n =2 from CuAu-I-like structure: I and II indicate, respectively, VFF and LAPW results described in text.

GaSb
Ga&AsSb3
Ga&AsSb
Ga4.As3Sb
GaAs

0.0
0.619
0.870
0.681
0.0

0.0
1.01
1.33
1.15
0.0

Cl eq

6.1068
5.9891
5.8786
5.7759
5.6816

82.147
89.138
96.373
103.789
111.177

37.377
41.381
45.864
50.855
56.311

five A4 „B„tetrahedra with n =0—4. Longer-range in-
teractions are treated in Ref. 60(a).
To calculate the interaction energies J (P) we note that although v7 (o) for an arbitrary configuration cr is

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900

800-
hC

700-

CO

0

CL 6O0-
E
500-

—Sulk Cup & Au&

—Anharmonic
p

= CuAur —Harmonic

4O0 ~' I
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
Cu Atomic Fraction x Au

FIG.

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I I I

(a) as=a«[GaSb]

asAsxSb1-x
Set I
1400 K

Epitaxial

alloy +.-..-
..

''

.~~ Epitaxial
constituents

which depend on (x, T) [see Eqs. (2.14) and (2.2)]. How-ever, Eqs. (3.10)—(3.15) permit explicit calculation of

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(iii) The cluster approach can readily distinguish
among competing phases at (x, T) on the basis of the
different statistical and structural properties of each
phase. For alloys of lattice-mismatched constituents we
expect simple trends in the relative energies of ordered
compounds and disordered alloys (bulk or epitaxial). For
example, at T=0 we note that for an ordered compound m, P„=5„and Eq. (3.7) [(3.8)] reverts to Eq. (3.9a) [3.9b)], except that the last terms in Eqs. (3.9)—due to distortions because a cluster is embedded in an alloy environment —vanish

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900

800—

I

a = CU3AU

T = 689.3
x = 0.267

I I I

P

= CuAuI
T = 713.1
x = 0.499

I I

[Bulk Cuq „Aux

700-

600—

500—

400
900

(b)
800-

700—

600-

T = 708.6
x = 0.261

= 744.9
x =0496

Epitaxial Cuq &Au&
a& = aeq(CU)

T = 460.3
x = 0.717

500-

Cl

400
e 900
c

CL 800- I
700—

T = 666.6

T = 7110
x = Q.496

I I I

Epitaxial Cuq „Au„
a, = aeq(CUALlI)

600— 3.5

31

500 " D

400

(d)
800-

700-

T = 696.1

T = 626.9 x = 0.496

x

— 0 266

Epitaxial Cuq „Au~
a, = a~{AU)

600- T = 535.2
x = 0.734

500-

400
0.0
CU

Q. 1 0.2 0.3 0.4 0.5 0.6 0.7 Q.8
Atomic Fraction x

D

0.9 1.0

Au

FIG. 7. Phase diagrams for Cu& „Au in bulk, (a), and epit-axially for [001] substrates with a, =a,q[Cu], a,„[CuAu-I], and a,q[Au], (b), (c), and (d), respectively. Shaded areas indicate
single-phase ordered compounds; asterisks in (b)—(d) indicate
bulk order-disorder transition temperatures.

2. GaAs„Sb&

The cluster description described above also applies to the ternary clusters A4 „B„Crelevant to pseudobinary A] B„Calloys. These clusters may be taken from ter-nary Landau-Lifshitz A4 „B„C4structures analogous to those for binary compounds above: a CuAu-I-like ABC2
structure

"

and the "luzonite" structure

"

for A3BC4
and AB3C4. Each ternary structure has, in addition to the unit-cell lattice parameter a and a tetragonal dimen-sion c, cell-internal structural parameters describing the positions of the atoms of the common C sublattice; see

Refs. 7(a), 8(b), and 60(a) for pictures of the unit cells and the structural parameters. These parameters must be re-laxed for each value of the external constraint (in bulk for fixed cell volume, and epitaxially for fixed a~l =a,). For
convenience we characterize these A 4 „B„C4 com-
pounds by cubic elastic constants, although they are strictly speaking tetragonal.
The parameters t

b,H„ I were determined in two
different ways, which illustrate the crucial role played by
the purely cluster property AH„, absent entirely from phenomenological descriptions:
Model I: EH„ from ualence force field. First-principles
calculations of the total energy, using the full-potential
linear augmented-plane-wave (h46 Tf 389 228.89 332.11 Td254.56 Td (in

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I r I 1 I I f I

1400-~ ~ Bulk GaAs„sb, „T= 1245

I

rr = 0.482
1200
1000
800
600

1800
1600
1400
1200
1000

I

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LAP W predicts AHbk =

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TABLE III. Bulk (AH») and epitaxial (6H,~) excess enthalpies and disordering energies AEd;, (kcal per mol fcc sites) for Cu4 „Au„ordered compounds at (T=0) and disordered Cu] „Au alloy (at
T =

EPITAXIAL EFFECTS ON COHERENT PHASE DIAGRAMS OF ALLOYS

(b)

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Moreover, as discussed in Sec. IIID, the CuPt ordering
most frequently observed is probably catalyzed by sur-
face effects not explained by our approach. Interestingly,
ordering of In& Ga As grown by the near-equilibrium
LPE method near x=0.48 appears famatinitelike, in
qualitative agreement with the relatively large region of
stability of Ga4AsSb3 in Fig. 8. The presence or absence of a given ordered phase in the phase diagram may also
be modified by finite temperature effects: although ex-
pected to exist for all substrates on the basis of the T =0 epitaxial model I 6H,, Fig. 8 shows CuAu-I-like Ga2AsSb to be stable to T =0 for a, =a, [GaSb], entropy
stabilized for a narrow temperature range for
a, =a, [Ga2AsSb], and absent for a, =a, [GaAs]. Thus the T=O epitaxial formation enthalpies are only a guide to which phases may be present.

C. Modeling epitaxial distortions of phase diagrams

Thus far bulk and epitaxial 3, B alloys have been
described as a mixture of distorted clusters. Even when such clusters are undistorted their energies AH„
include +" ' '

an "elastic" contribution (associated with
compressing A and B to a„=a, [A 4 „B„]) and a
"chemical" contribution

EPITAXIAL EFFECTS ON COHERENT PHASE DIAGRAMS OF ALLOYS

TABLE V. e'"' (in kcal/fcc-site mol) and order-disorder temperatures (K) found from the e-G model under bulk and epitaxial [with a, =a,,

(x =0.5)] conditions; model I results are used for GaAs, Sbt „. Temperatures calculated within CVM are in parentheses.
T(2)

Bulk

Epitaxial

—4.2073

—4.1381

—5.6302

—5.5673

Cu[Au —3.9365

—3.8826

684.5

(689.3)
666.9
(666.6)

731.3
(713~ 1)
729.6

(711.0)

558.6

(536.4)
548. 1

(523.5)

Bulk

Epitaxial

—1.4569

—1.4297

—1.8335

—1.8215

GaAs] Sb —1.2925

—1.2971

262. 1
(270)
252.3
(252)

218.5
(217)
218.0
(218)

185.7
(180)
190.6

G, (GbI,). In Fig. 10 we show contour plots of the

relevant di6'erential strain energy

b,(a„x)=G,~(a„x)—Gbk(x) (5.10)' as a function of a, and x, for Cu, ~Au, [Fig. 10(a)] and for GaAs„Sb& [Fig. 10(b)], for either models I or II,

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induced shifts of the transition temperatures (calculated
within

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Examination of the cluster probabilities provides in-sight into how an alloy responds to the epitaxial con-straint. For high enough temperatures the cluster proba-bilities P„(x,T) assume their random (R) binomial distri-bution values. For our choice of clusters n =0—4,

P„(x,T)=4!/[(4—n)! n!]x"(1—x) (5.11)

As T is reduced the P„determined variationally from the cluster variation method depart from the random values, reAecting a thermodynamic enhancement or suppression of the distinct clusters. Figure 13 shows the excess clus-

tions of state in the cluster description) determined from LAPW calculations

"

produce good agreement with ex-

periment (QPk-—4.0 kcal/mol).] However, 0 at x =0 and 1 are almost identical for models I and II, emphasizing that EEs(a„x,T) [Eq. (3.14)] depends primarily on alloy elastic properties and only very weakly on the parameters AH„which distinguish the two models.

E. Cluster populations

ter probabilities b,P„(x,T)=P„(x,T) P—„(x) for bulk
(solid lines) and epitaxial (d'ashed lines) Cu, Au for the three substrates given in Figs. 4 and 7. While the bulk curves are indistinguishable from the anharmonic results of Refs. 60(c) and 60(d), the epitaxy-induced redistribu-tion of cluster probabilities is generally small over the en-tire composition range. At the lattice-matched composi-tion the bulk and epitaxial cluster probabilities are identi-cal for all clusters, so that bulk and epitaxial alloys are structurally and energetically indistinguishable.
The e-G analysis of Sec. VC may be used to under-stand these cluster redistributions. For e' ' &0, the prob-ability for cluster A4 B is enhanced

"over its ran-
dom value; under epitaxial conditions, if [Eq. (5.10)]
b e('(a,)= —b,(a„x) & 0, cluster m will corresponding-ly be suppressed with respect to bulk. Inspection of Fig. 10(a) suggests prominent suppressions near x =0.2 for the Cu3Au cluster on a, =a, [Cu], and near x =0.8 for CuAu3 for a, =a, [Au]. These expectations are directly confirmed in Figs. 13(a) and 13(c),respectively.,
In Fig. 14(a) we show the b,P„(x,T) for GaAs Sb, for a, =a,q[Ga2AsSb] at 1300 K, using model I; results

0.2

0.1

0.0

-0.1

'Pc 0)

Ec
CL

CL

0.1

0.0

Cu, „Au„, T=SOOK

I

(c3

as=aeq [Cu]

as=aeq [Au

1

0.2 —,

'

2 2 ..----.-''---'-

..

/

'.

0. 1 —:,:

/

p S

~ X ~ GaAssSbt
5. -0.2
-0.3-

-0.4- =1300K i

GaAs4+

I I I I I

0.3 0.4 0.5 0.6 0.7 0.8 0.9

-0.5
0.0 0.1 0.2 1.0

Q.06
Q.05
0.04
0.03
0.02
~ 0.01
0.00
-0.01
-0.02
-0.03

-0.04-- IT 1300K I
0Q5 i
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 Alloy Composition x

I I I I I I I I I

GaSb 8ulk Alloy Composition xb„,„(p.) GaAs 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

m BT /Xi1Xi17 7.53 Tf 415.89 298.11 T1 (0.)Tj2T BT /Xi1ET BT /Xi17 7.51 Tf 461.67 /Xi17 8T4.31 Tf 1 Td (8)1 Td (ctiv8.86 Tf 258.67 136.56 Tdd (I)Tj ET B Tf 365.67 760.22 T1ET BT d nharmonic /Xi17 8.01 Tf 340420.22 T6T d0Sbt)Tj ETFIGET BT /Xi17 8.86 Tf 414.28 (0)Tj0Sbt IbT T /Xi17 9.15 Tf 473343.11 82 Td -ial (X)Tj 6 (variati(,)Tj ET BT /Xi17 9.75 Tf 322 297 550.78 (0.)T23 Td (of)FIGET BT /Xi17 8.86 Tf 378 545(0.)T23 t)Tj ET1T /Xi17 9.45 Tf 14 487.78 Pc d ET BT /Xi17 9.55 Tf 97.11 6986(Td (I)Tj Ej ET BT /Xi17 9.2 Tf 381.5310.78 Td (8Tj ET BT ET BT /Xi17 6.89 Tf 17645.67 Tdd (8Tj ET BT Tj Ej ET BT /Xi17

and

depart(BT /Xi17 9.04 Tf 528.8 614.447.56 Td1(random)TjIBT /Xi17 9.26 Tf 396 4.447.99j ET1(and)T BT /Xi17 8.86 Tf 4557.78 Td BT j1(and)TT BT /Xi17 8.64

00 (ET BT)Tj ET BT /Xi17 9.j ET BT06.8.8 Tdj0Sbt 00 (ET BT)Tj ET BT /Xi17 9.85 Tf 4287.78 677.56j E10rmonica/Xi17 7.8 Tf 104 13689 474.18 Tdj0Smonica. 53T j0SbAs

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using II are similar. Although Cu] Au has stable clus-
ters (AH„&0) while GaAs Sb, does not (bH„)0),
both show enhancement of mixed clusters (e' '&0), as
discussed in Sec. VC. The e-G analysis using Fig. 10(b)
predicts [as confirmed in Fig. 14(a)] for a, =a,q(x =0.5)
an epitaxial suppression of Ga4AsSb3

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either in phenomenological el '

e astic descriptions or in
rs -principles cluster-based calculations.s. Thisis depen-

between alloy constituents, refm. ecting different
on engths and their imperfect accom-
mo ation in an alloy environment.

C. Quantitative results

1. Separating alloys

Using model I data, used to corn ute

results for substrates lattice a;matched to the al-

results for II

xpected to be similar (within -6% becau
similar epitaxial su res

'

s pp ss ons o t iscibihty g ps}.
e epitaxy-induced increase in dIM/dx =d b,F/d x (i.e.,
g. ',aj is most pronounced at x =0.5
given p (fixed growth conditions) corresponds to diffe ~ ~

LM

values of x, and x. F'

s o i erent

ep

x Qk igure 1 5(b} shows strong devia-
tions from x, =x (i.e. =1
and 50 Ca p Qk

=) even well away from x
d bove the calculated maximum b lk

+LM

gap temperature (=1245 K). Th 1

m u miscibilit
ese results are directly

relevant to liquid- hase e

'

'q '

-p ase epitaxy and strongly resemble the
original curve of Stringfellow
In Fig. 14(b) (discussed in Sec. VE) we dis la

matched to x =0.5. Alon

IM P„—p versus xI,I, (IM) on a substrateealatt'ice
one among the five clusters the
nearly lattice-matched GaAs a szSb 1 2 c uster is enhanced

text of corn

over the entire composition range. In th e con-
omposition pinning we note that the po
ic t e probability redistribution for
a s2 z

clusterss is a maximum correspond rou ghl
gni cant composition pinning in Fi. 15 Figure 14(b) is thus a mic
heno

a microscopic manifestation of the
p enomenon of composition pinning.

2. Composition pinning in ordering alloys
and ordered compounds

The qualitative remarks above hold o for ordering

e.g., Cu, „Au„] or phase-separating x, e.g., most isovalent semiconductor] allo s.

~ince formally the miscibilit - a

a oys.

' '

i y-g p temperature is negative
or or ering alloys, we expect considerably less corn osi-
tion pinning for ordering alloys. In Fi. 16

' '

n pinning curves for the disordered Cu A
alloy and ordered Cu

ui-x ux
dered

dere]

t2ay

1singb}

pin154jj ET BT /Xi19 10.33 Tf 395. 477.3 Td (154jj ET BT/Xi19 8.28 Tf 194478 678.8i-)Tj17 Td (T BTC/Xi19 9.61 Tf 206.64 657.7 Tj E16%)Tj ET B /Xi19 10.33 Tf 39.33 586.3 Td (16%)Tj ET B Xi19 5.79 Tf 348 428.67 8 T ET

1

1ord Tf 0 Td8TTj ET BT /Xi19 6..33 a2Tj ET Kj E65/Xi19 1 Td (')Tj ET BT 22.54 7n33 586.4j E65/7sing 16% i11(dj ET BT /Xi19 10.33 Tf 39767 700.1T19ET 11(dj ET BT4885 /Xi19 8.

in

dIM/ch56 TXi19 5.21 Tf 168.44 Xi19 1d (pha7 („Au„])Tpot Td 536.44 Td (2.)Tj h4T13 Tf195.11 78 Td (or)(bT /Xi19 9.26 Tf 405.152 481.4.56 Td T%)Tj ETiBT /Xi19 13.67 Tf 1.26 Tf Xi171.67 Td (p/Xi19 6.84 Tf 251 717n33135

or

dIM/s:9 9.26 Tf 428 63689044 55004 7261..44 482 (t2ay)Tj ET B/Xi19 9 8.73 T192.8 71.d (or)T„Au„e

a) ET BT /Xi19 11.551 6Tj E535Td (')

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substrate lattice matched to ordered CuAu-I, using CVM
results.

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Molecular-beam epitaxy (MBE) is frequently regarded as a nonequilibrium or kinetically controlled process. However, recent work suggests that provided the ac-tual reactions occurring are known and characterized by their thermodynamic variables, an equilibrium thermo-dynamic analysis can account for observed growth rates and other properties of epitaxial alloys. Seki and Kouki-tu (SK) have recently given such an analysis of molecular-beam epitaxy growth of bulk III-V pseudo-binary alloys, neglecting the strain effects of coherent epi-taxy we have considered

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rAIAs /rinAs

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TABLE VI. Equilibrium lattice parameter a,q

{A) and cubic
elastic moduli C;J (GPa) used for elastic thermodynamic description of MBE growth of Al„ In, „As. Interaction param-eter 0=2.4964 kcal/mol. Data taken from Ref. 78.

A1As
InAs

aeq

5.6622
6.0584

120.2
86.5

57.0
48.5

C44

58.9
39.6

stituents are given in Table VI; the parameters of the equilibrium constants for reactions Eqs. (7.2a) and (7.2b) are given in the first two rows of Table VII. Figure 18(a) shows the In incorporation coeKcient under bulk and ep-itaxial conditions for two different vapor-phase composi-

tions x„,but with the same net group-III applied pres-sure P;f', =1 X 10 Torr and Pg

=5 X 10 Torr. Over

this temperature range the Al incorporation coefticient, as mentioned above, differs imperceptibly from 1. Figure 18(b) shows the bulk and epitaxial steady-state alloy com-positions for a variety of x„values. In all cases at xzM bulk and epitaxial curves coincide, but there are significant modifications away from xLM. In Fig. 18(c) we display composition pinning curves, obtained by plot-ting the steady-state alloy composition x&k of the bulk al-loy against that for the coherent epitaxial alloy x,. Un-like the CVM results shown in Fig. 15, which are directly relevant to experimental liquid-phase epitaxy (LPE) re-sults, the degree of composition pinning in MBE depends on an external constraint, i.e.,

the vapor-phase composi-

tion x„.Increasing the total

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Set

I
II
III

[001]
substrate

InP

QaAs
QaAs

papIn

0.16
0.16
0.08

PA1

0.148
0.373
0.187

pap =4pap As As4

92
92
92

TABLE VIII. Experimental conditions for data sets I—III of Turco, Guillaume, and Massies (Ref. 78). Partial pressures in units of 10 Torr.

Once again the agreement is quite satisfactory given the uncertainties in the input parameters of the calculation and the sizable error bars of the experiment. The similar-ity of epitaxial and bulk curves indicates that most

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is converted to [a(x)

—a,]/a„ the unstrained value, and (ii)
one corrects for extra strain introduced by cooling from
growth to room temperature. The magnitude of b,a~/a, is
then consistent with composition pinning.
8M. Kume, J. Ohta, N. Ogasawara, and R. Ito, Jpn. J. Appl. Phys. 21, L424 (1982); H. Asai and K. Oe, J. Appl. Phys. 53, 6849 (1982); K. Oe, Y. Shinoda, and K. Sugiyama, Appl.
Phys. Lett. 33, 962 (1978); A.

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nary compounds subject to the epitaxial constraint the {1,4,6,4, 1)-fold binomial distribution degeneracies [Eq. {5.11)] of A4 „B„Cclusters are also broken to an extent measured by (C3$/C» —1), which we thus neglect.
S.-H. Wei, H. Krakauer, and M. Weinert, Phys. Rev. B 32, 7792 (1985).
P. N. Keating, Phys. Rev. 145, 637 (1966); R. M. Martin, Phys. Rev. B I, 4005 (1970).
'M. F. Gratton and J. C. Woolley, J. Electron. Mater. 2, 455 (1973); J. Electrochem. Soc. 127, 55 (1980). See also J. R. Pessetto and G. B.Stringfellow, J. Cryst. Growth 62, 1 (1983). This omitted chemical term raises the b,H„with respect

binomial