PHYSICAL REVIEW B VOLUME 38, NUMBER

EPITAXY-INDUCED STRUCTURAL PHASE TRANSFORMATIONS 10 125

10
U

I
5

fh

CL

p

0.5

CdTe

Q 4

g 0.3

gy) 0.2

C

m p~

Q.O
45 50

i I I 4 ~ I ~ ~ ~ ~ j I i I i

55 60 65 7Q 75
Volume (As)

0.5

I p4
CL

~ 0.3

cn 0.2
I

C

LU p~

a face-centered square lattice. Second, the unconstrained c axis, perpendicular to the interface, is free to relax. This

reduces the energy of the epitaxial phase relative to the hydrostatically compressed phase

10 126 SVERRE FROYEN, SU-HUAI WEI, AND ALEX ZUNGER

TABLE I. Static structural properties of CdTe, MgS, and NaCl in the indicated structures. ao is the equilibrium lattice constant, Bo the bulk modulus, ~the minimum energy measured from the ground-state minimum, and E, is the cohesive energy. All energies are per two atoms. The zero-pressure ground-state structure is indicated with an asterisk. CdTe and NaCl experimental lattice constants and bulk moduli are low-temperature all others are room-temperature

Structure

Qp

(GPa) (eV) (eV)

CdTe B3' Theory
Expt.

NaCl5 667429.Td (5p)Tj E6 BT /Xi2 8.23 92 , 27pt. modu5 490.TheTd (the)Tj 5 BT /Xi2 8.42 Tf 46odu5 497.72eTd (Theory) BT /Xi2 9.58 Tf 177.99 635.89eT89.All

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i.~ —
(a)
1.0

0g. B1

o.5- (b)

83

I i I

NaCX

1.1 -(a)
u 1.0
0.9—

I ~' I
B3

as 0 4-
CL

0'
0.3-

Q) 0.2-
c
LLI

—C-
II

B1
8$

'co 0.4— Ch.
o 0.3—

C5

0.2—
C
LU

0.1—

0.0-

5.4 5.6 5.8 6.0 6.2 6.4
Lattice constant {A}

6.6
5.0

I I I

5.2 5.4 5.6
Lattice constant

5.

8

5.

5.

5. . as0. B15.

83 as

5. assubstrate(-(a))Tj ET BT /Xi3 4.4220f 345 77 713.9lTd (Lattice)Tj ET BT /X2 12.88 Tf 248 776555.87parameterTd (5.)Tj ET BT /X26 8.8.55i3 5.14 608.78Solidd (5.)Tj ET BT 7f 478.871f 160.14 608.78andd (5.)Tj ET BT /Xi3 7.98/X13 0.14 621.66dashedd (5.)Tj ET BT 7f 11.58 7f 1 5. 83as5.

B15.83as. substrate(-(a))Tj ET BT /Xi3 4.447/Xi3 0 0f 602.68lTd (Lattice)Tj ET BT /Xi3 9.33.13 620 0f5660.59parameterTd (5.)Tj ET BT /X21 8.83 Tf 2483.9 08.78So 5. 83asC5 20.

{A} o2as83as5. 0- 2Lattice o

83