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Effects of ordering on the electron effective mass and strain deformation potential in GaInpz.. Deficiencies of the k p model

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The conventional eight-band k p model predicts a dec~ease of the electron effective mass and no depen-
dence of

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where E

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from the LAPW band-structure using a simple finite-
difference scheme. We estimate the numerical error in-
volved in the effective mass and deformation potential
calculations to be smaller than 1%.
The effective masses calculated within the LDA are
affected by systematic errors, rejecting the well-known
band-gap underestimation of LDA. For example, our
LAPW calculated electron effective mass of InP is

m,&=0.034mp, compared to the experimental value ' m,&=0.076mp. In the case of GaAs, the LDA effective
mass calculated by Christensen is m,&=0.012mp, while
the observed value '

is m &=0.067mp. Note, however,
that the LDA errors are expected to cancel to leading or-
der when we consider the effective-mass difference be-
tween the disordered Gap 5Inp 5P alloy and the ordered CuPt structure. The LDA effective mass of the disor-

dered alloy (rt=0) is approximated by the average of the
effective masses of pure GaP and InP, calculated
at the substrate lattice constant a,: m z D&(0}
=1/2[mo,

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0.13

LDA

0.11

0.09

0.07

[111] [101]

0.0 0.5

Ordering parameter

1.0

FIG. 1. Electron effective mass in the ordering direction [111]and in the perpendicular direction [101],as a function of the ordering parameter g. The k p effective masses are ob-tained from numerical diagonalization of the 8X8 k.p Hamil-tonian, while the LDA effective masses are calculated using Eqs. {4)and {5).

cussed the ordering-induced anisotropy of the hole

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V
O
- 7.0

~ 0'pf

0.0

LDA

0.5

Ordering parameter q

1.0

The LDA and k.p band-gap deformation potentials for
(001) epitaxial strain are compared in Fig. 2 as a function
of the ordering parameter g. Since the I.„deformation
potential of the dis.33 6 /Xi4 9.17 Tf 386 671.44 T6 681.56 Td (g.)Tj - 9.42 T

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and orderinga

„deformation Tf1 /Xi4894.78 53T2.67mix Td (parameter)Tj Xi45T /Xi4 7 64457428 T2.67Td (the)Tj ET BT /XT BT /X23 70428 T2.67 Td (ordering)Tj

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compared Epf 5

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