IIII..O I Ir r Ir 1

r IIr iI ~ ~

II II jp rr re,

PHYSICAL REVIEW B VOLUME 30, NUMBER 10 15 NOVEMBER 1984

Bond lengths around isovalent impurities and in semiconductor solid solutions

Jose Luis Martins and

6218 JOSE LUIS MARTINS AND ALEX ZUNGER 30

tal. Hence, rather than assuming that bond lengths are
transferable, in the manner of Pauling, we assume instead
that bond densities and their attendant elastic response
are transferable (i.e.

,

independent of their environment).
Whereas the true charge density pec[AC:8] of the impurity
BC bond can differ substantially from that of the AC host density it replaces, (i.e.

, /sp~

=pec[AC:8]

—pqc[AC] can be
a large perturbation), we expect pec[AC:81 to be closer to
the density psc[BC] of the BC bond in the pure BC system (i.e.

, Ap2= psc[AC:8]

—peg[BC] is

a smaller perturbation).
Neglecting the small density perturbation Ap2, the change in
elastic deformation energy

U induced by the insertion pro-
cess can be modeled by a valence force field (VFF), general ized to have the appropriate force constants for each kind of bond, e.g.

,

the VFF of Keating "2

4

U=

$ $,u[r (i, 1)

r (i, 1)

—d2)2
m=

1 8d
2

3

4

d '

+$

g

g

g 2P

r (is) r„(is)+, (2)

I s= 1m=

1

= +1

where

d

=8;, is the equilibrium interatomic distance,
r (!,s) is the vector connecting atom

s in unit cell

i to its

mth nearest neighbor, and

u and

P are the bond stretching
and the bond-bending force constants, respectively. The
first sum in Eq. (2) extends over all nearest-neighbor pairs, whereas the second sum extends over all bond angles
around every atom. For this AC:8 impurity system, we
describe the

B

—C bond around the impurity using the
parameters use, Psc, and dec taken from the pure BC crys-tal, P' and dqcdec are used for the 8—A —C bond bending, and the constants uqc, Pqc, and de, which are taken from the pure AC crystal, are

e

30 BOND LENGTHS AROUND ISOVALENT IMPURITIES AND IN... 6219

TABLE II. Predicted impurity BC bond length R =R~~~.~ (in A)
for an isovalent B-atom impurity in an AC host crystal and the re-
laxation parameter e [Eq. (1)].

System R (A) System R (A)

A1P:In
GaP:In
A1As:In
GaAs:In
AlSb:In
GaSb:In
A1P:As
AlP:Sb
AlAs:Sb
GaP:As
GaP:Sb
GaAs:Sb
InP:As
InP:Sb
In As:Sb
ZnS:Se
ZnS:Te
ZnSc:Te
P-HgS:Se
P-HgS:Te
HgSe:Te
ZnS:Hg
ZnSe:Hg
ZnTe:Cd
ZnTe:Hg
y-CuC1:Br
y-CuC1:I
y-CuBr:I
C:Si
Si:Ge
Si:Sn
Ge:Sn

2.480
2.474
2.553
2.556
2.746
2.739
2.422
2.542
2.574
2.414
2.519
2.564
2.595
2.700
2.739
2.420
2.539
2.584
2.611
2.716
2.748
2.482
2.587
2.755
2.748
2.440
2.563
2.585
1.665
2.380
2.473
2.549

0.65
0.63
0.60
0.62
0.61
0.60
0.65
0.61
0.60
0.62
0.57
0.60
0,67
0.60
0.64
0,70
0.67
0.71
0.76
0.71
0.74
0.73
0.74
0.70
0.69
0.81
0.80
0.79
0.35
0.58
0.53
0.55

InP:Al
InP:Ga
InAs:Al
InAs:Ga
InSb:Al
InSb:Ga
A1As:P
A1Sb:P
A1Sb:As
GaAs:P
GaSb:P
GaSb:As
InAs:P
InSb:P
InSb:As
ZnSe:S
ZnTe:S
ZnTe:Se
HgSe:S
HgTe:S
HgTe:Se
rg-HgS:Zn
HgSe:Zn
CdTe:Zn
HgTe:Zn
y-CuBr:Cl
y-Cur:Cl
y-CuI;Br
Si:C
Ge:Si
o.-Sn:Si
a-Sn:Ge

2.414
2.409
2.495
2.495
2.693
2.683
2.395
2.444
2.510
2.387
2.436
2.505
2,562
2.597
2.667
2.367
2.407
2.502
2.553
2.579
2.665
2.380
2.494
2.674
2.673
2.367
2.407
2.S00
2.009
2.419
2.645
2.688

0.73.
0.73
0.74
0.73
0.75
0.74
0.67
0.73
0.71
0.68