Phystca l17B & IISB (1983) 185-187
North-Holland Publtslurt8 Company 185

ELECTRONIC STRUCTURE OF SUBSTITUTIONAL 3d TRANSITION ATOM IMPURITIES IN SILICON

A. ZUNGER and U. LINDEFELT

Solar Energy Research Institute Golden, Colorado, 80401 USA.

We report the results of a self-consistent calculation wlthin the local denslty approxlmatlon for all the substltutlonal 3d transition atom (TA) impuritles In an extended silicon host crystal uslng the quasi band Green's functlon method. Chemical trends in the gap state enerqles and 3d-llke resonances are discussed as well as trends in the effectlve electronlc configuration of TA impur~tles. An explanation for the remarkable property that many dlfferent charged states of TA lmpurlties exlst in the narrow band qap, despite the fact that the corresponding ionized states of the free TA span a ranae of ~ 60 eV, is proposed.

186 A Zunger, U Lmdefelt / Substztuttonal 3d transttton atom tmpuntles m Sdwon

t= Threshold-] -e Threshold
z n ~ ~ c, v T,

/ 1
ILl_ s

- 10

- lZn Cu NI Co Fe Mn Cr V Ti FIGURE 1.

A
o

~ 1.2
O} 1.0
(~ 0.8
00.6
"~0.4

02'

~i 0.0

% l I ' l ~ I I I

. ,~%zV"

12
11
10
9
8
7
6
5
~4

'3

ZnCu Ni Co FeMn Cr V Ti
FIGURE 2.

3e etc. indlcates the gap level occupatlon for the neutral state of the impurlty.

The major localized defect level of highest energy is the t 2 dangllng bond hybmd (DBH), appearlng for Sl:Zn just above the valence band maxlmum and dlsappearing into the conduc-tion bands for Sl:CO. The ~=I component of the t2-DBH wave functions Is qualitatwely charac-

Defect Charge Qnet (e)
0S 00 -05 -10

b) o
80 - 2~

U d o
0 ~gap"-" >,

• t-
o • W

• Q ,0
,= •

t i

'I I I I'

(a) ,.,
~gap • o ,...,

4)
O
,51Q

o QVB-"-" "

o O

2O | 315 1_ 40 2.5 30 40
Gap Level Occupation
FIGURE 3.

A
o

"~7.~

.~-- 0

~rc

e
O
i-
i

O3

m J¢ O
2.

0 0

teristic of a host-llke dangllng bond (vacancy) wave function. However, a

A Zunger, U Lmdefelt / Substttuttonal 3d transmon atom impurities tn Silicon 187