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Metastable impurities in semiconductors: Si:Mg and Si:Be

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Using 30-year-old ideas on Fermi-energy- (sF) induced stability enhancements in impure semi-conductors, it follows that if two impurity sites with different electrical levels exist, one can expect to find, inside the band

34 METASTABLE IMPURITIES IN SEMICONDUCTORS: Si:Mg... 7453

Nlg Be
unrNaxed relaxed unrelaxed relaxed

3.5

Al
~l

LLI

CP

s

LU
lO

0
2
Nle
Atom

C)

C
Lal

2.5
t-

(0/-)

l

Mg;

Mg I /'(0/+)

0-

Be,8i

Mg,. i

r

2 0

c

FIG. 2. Calculated total energies EI V] for neutral impurities in Si. S, TI, and HI refers to substitutional, tetrahedral intersti-tial, and hexagonal interstitial, respectively. STS; is a substitu-tional impurity next to a Si tetrahedral interstitial, 8 is a bond-centered impurity (with the two neighboring Si allowed to relax along the (111) direction to their mirror image position), and ST~ refers to a substitutional M next to a tetrahedral interstitial M. Also shown are the ground-state impurity atomic energy (Atom) and the energy of the bulk silicide M2Si. The free metal is chosen as the zero of energy.

Mg. /
/

I

1.5 I (Ev+Ee }/2

/

1 I 1

0 0.1 0.3 0.5 0.3 O.i 0

F„Fermi I evel & E, F
FIG. 3. Total energy diagram for the various charge states of substitutional (S) and tetrahedral interstitial (i) Si:Mg, using the band gap as the unit of energy.

silicon; Mg impurities are also less stable than the free im-purity atom plus silicon, whereas the converse is true for

Be impurities (except site 8), (ii) when a S and a TI im-purity are placed next to one another, the stability is enhanced considerably relative to the isolated pairs (by 1.25 eV and 1.4 eV for Be and Mg, respectively), clarify-ing the reason why these impurities tend to aggregate (un-less special