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function matrix and the diagonal potential matrix in terms of these MTB bands and solves for the de-fect energies e;(hV, MTB) and wave functions I(;(h, V,Mrs) in the standard Slater-Koster
fashion. The defect wave function is hence spectrally constructed from host band wave func-tions extending up to the energy e,„,(MTB) of the highest (MTBth) host band included. The cutoff energy e«,(MTB) does not correspond

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a.u. (half a Si—Si bond length), one finds from Fig. 2 that the known unrelaxed Si vacancy tz en-ergy e2——0.7 eV (Refs. 3 and 4) is mapped" into the square-well model by taking Vo ' ——2.375 Ry. One hence finds that an impurity with radius

Ro =3 R.U.)&0 w111 have its energy level e&

above eq (e.g., e&——1 eV for Vo" =0.875 Ry) even if its potential amplitude Vo" is smaller than Vo '. Hence, a large size impurity atom having a shallow potential well can form acceptor levels above the host vacancy level, if the host atom is sufficiently small. This clearly does not support the TB notion that "weaker" impurities will have their energy pinned below that of the "stronger" impurities. The physical reason behind this observation is simple: in the TB model the defect is character-ized by a single variable; the difference
A V~@——V —Vpp between diagonal TB matrix ele-ments of the impurity and the host atom being re-placed. Except in the work of Ref. 8, the diagonal elements V«and V~p are not fixed uniquely by the fitting procedure of the band structure since the latter is invariant (up to a constant related to the host's work function) under constant changes in I V;;I. In a more complete model, however, the perturbing potential is characterized by a continu-ous function b, V(r) and a complete basis set

I ~ a) I. The physically relevant characteristics of
b, V(r) are then reflected in two coordinates rather than one: the radius Ro and the potential strength Vo. [This information is contained in the matrix

representation (a ~

b, V(r) ~ P) if the basis I ~ a) I

is

complete in the domain of EV(r), but not if it is

grossly in/Xi2 9.08 Tf 87.27 376.74 329.3 Tt18.00.2f 149.77 317.5 Tdif

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