SYMMETRIC RELAXATION AROUND INTERSTITIAL 3d IMPURITIES IN SILICON

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Abstract: EPR studies suggest that most transition atom impurities in silicon occupy the tetrahedral interstitial (TI) site, preserving the T_d symmetry of the host (1). In this paper we will give, within the local-density approximation, a unified description of the electronic structure and "breathing-mode" relaxation of tetrahedral interstitial Cr, Mn, <u>para na misiwa manatatan in kuthoniti na </u>

I. ELECTRONIC STRUCTURE

The electronic structure before relaxation has been calculated self-consistently

with EPR data (maximum spin). Ni is seen not to introduce any gap states, and is thus

Fig. 2 shows examples of the radial components $\Delta \rho$ _o(r) in a Kubic harmonics expansion of the impurity-induced change in charge-density $\Delta \rho(\vec{r})$:

$$
\Delta \rho(\tilde{r}) = \frac{\Sigma \Delta \rho}_{\ell}(r) K_{\ell}^{a_1}(\tilde{r}) , K_{\ell}^{a_1}(1,1,1) \geq 0 \qquad (1)
$$

The shape of $\Delta \rho_0(r)$ around the first and second nearest neighbours (1NN and 2NN) is depicted in Fig. 2b. As will be seen below, the position of 1NN and 2NN in the antibonding region (negative $\Delta \rho_{\Omega}(r)$) largely determines the relaxation pattern. The radial

host charge-density around the TI site (dashed lines). Apart from the large peaks in the $l=0$ and $l=4$ components, which are both inside the impurity core, there is a rather weak tendency to displace charge from the neighbouring host atoms towards the impurity, and this is effected mainly through the spherically

2NN. The nodal structure in the projected density for the 2NN, responsible for the different directions of distortion of INN and 2NN, is found to be related to the position of the atoms in the antibonding region:

 t the projected density has a node as in Fig. 5b if the as in \mathbb{R}^2 atom is located to the minimum in t

density is nodeless otherwise. The effect of the aniso-[~]**0..** tropic components in L-lp(\sim) is to produce a small interaction and \sim - **2.QL-...LL.....L.-L.-...L....--'---'** force on both shells. This contribution is, however, on the INN. For more distant atoms, L'lF turns out to be negligible, so these atoms have moved only because of the source of the source of the source of the source of t
In the source of the sourc the displacement of the first two shells of atoms. the fourth shell is that the 4NN atom at a/2 (α), α (α), α for instance, is directed to the INN atom at tax \mathcal{L} is also the direction of distortion of the two atoms. This bond is thus compressed only slightly, typically around 1% of the bond length. If one is the bond length. If one is the first two distinctions of the $\mathbf{1}_{\mathbf{1}}$ ing between shells leads to a displacement which is a displace about 2/3 of the unconstrained displacement. REFERENCES Fig.5. (a) Host pseudopoten- $\frac{1}{\sqrt{2}}$. (b) The mag-axis (I) E.R. Weber, Appl. Phys. A30, I (1983). sity. (c) The integrand in (2) U. Lindefelt and A. Zunger: Phys. Rev. B26, 846 Eq. (4). The Si atom is at (3) A. Zunger and U. Lindefelt, Phys. Rev. B26, 5989 (4) U. Lindefelt, Phys. Rev. B28, 4510 (1983). $\mathcal{L}(\mathcal{S})$ u. Lindefelt and $\mathcal{L}(\mathcal{S})$ u. Lindefelt and $\mathcal{L}(\mathcal{S})$ (for \mathcal{A} , \mathcal{A} ے ق (7) J. Harris and R.O. J. Harris a
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