Department of Theoretical Physics
University of Lund
Sölvegatan 14 A, S-223 62 LUND, Sweden

Alex Zunger
Solar Energy Research Institute
Golden, Colorado 80401, U.S.A.

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,

J. D. Chadi et al. (eds.), *Proceedings of the 17th International Conference on the Physics of Semiconductors*

I. ELECTRONIC STRUCTURE

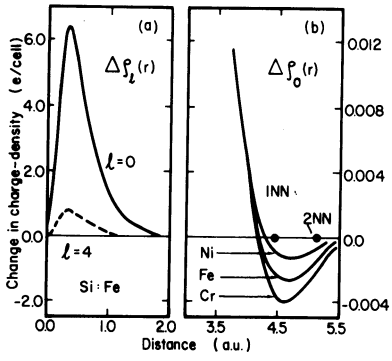


Fig. 2 shows examples of the radial components $\Delta\rho_\ell(r)$ in a Kubic harmonics expansion of the impurity-induced change in charge-density $\Delta\rho(\bar{r})$:

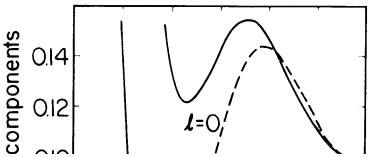
$$\Delta\rho(\bar{r}) = \sum_\ell \Delta\rho_\ell(r) K_\ell^{a_1}(\hat{r}) \quad , \quad K_\ell^{a_1}(1,1,1) \geq 0 \qquad (1)$$

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 $\Delta\rho_0(r)$) largely determines the relaxation pattern. The radial

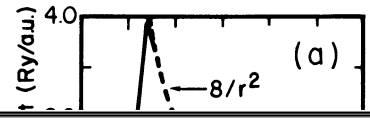
Fig. 2 Charge-density

ted at the origin.

in Fig. 3 for the representative case Si:Fe (solid lines) together with the radial components of the



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 1NN and 2NN, is found to be related to